

201-14485



NCIC HPV

Sent by: Mary-Beth
Weaver

05/22/2003 01:23 PM

To: NCIC HPV, moran.matthew@epa.gov

cc:

cc:

Subject: HPV registration number



John Heinze <jheinze@johnadams.com> on 05/20/2003 03:32:27 PM

To: Rtk Chem/DC/USEPA/US@EPA, oppt.ncic@epamail.epa.gov
cc: Amy Benson/DC/USEPA/US@EPA, Richard Hefter/DC/USEPA/US@EPA

Subject: HPV registration number

The LAB Sulfonic Acids Coalition is hereby submitting a robust summaries dossier (IUCLID Data Set), Assessment Plan and Data Matrix (summary table) for the Linear Alkylbenzene (LAB) Sulfonic Acids category of materials under the U.S. Environmental Protection Agency's (EPA) High Production Volume Chemical (HPV) Challenge Program.

LAB Sulfonic Acids are intermediates in the production of linear alkylbenzene sulfonate (LAS), a category of materials undergoing review in the OECD SIDS program with the US EPA as the country sponsor, and targeted for presentation at the OECD SIAM 17 meeting in November 2003. Since LAS is referenced as a supporting substance in the LAB Sulfonic Acids documents, this submission has been copied to Ms. Amy Benson, who is the EPA point of contact for the LAS review.

The LAB Sulfonic Acids Coalition believes that the current documents meet the requirements of the voluntary HPV Challenge Program and that additional animal testing would not provide significant new information useful in decision making.

If you have any questions regarding the assessment plan or the robust summaries, please contact me at 202-737-8400 (telephone), 202-737-8406 (fax) or jheinze@johnadams.com (email).

Sincerely,

--John E. Heinze, Ph.D.
Manager, LAB Sulfonic Acids Coalition
Senior Vice President, Science
John Adams Associates Inc.
529 14th Street, NW, Suite 655



Washington, DC 20045 Final Dossier Mar27 (1).pdf



Final Assessment Plan 5-20-03.doc



Final data matrix.xls

2003 MAY 22 PM 3:37

RECEIVED
OPPT CBIC

**Assessment Plan for the Linear Alkylbenzene (LAB)
Sulfonic Acids Category
in Accordance with the USEPA High Production
Volume Chemical Challenge Program**

Prepared for:

The LAB Sulfonic Acids Coalition

May 20, 2003

THE WEINBERG GROUP INC.

1220 Nineteenth St, NW, Suite 300
Washington, DC 20036-2400
e-mail science@weinberggroup.com

WASHINGTON
NEW YORK
SAN FRANCISCO
BRUSSELS
PARIS

TABLE OF CONTENTS

EXECUTIVE SUMMARY	1
INTRODUCTION	1
IDENTIFICATION OF STRUCTURE BASED CATEGORY	2
Relationship of US to European LAB Sulfonic Acids.....	6
Relationship of LAB Sulfonic Acids to LAS	8
Use Patterns and Exposure Potential	8
COLLECTION OF UNPUBLISHED AND PUBLISHED DATA	9
EVALUATION OF DATA FOR QUALITY AND ACCEPTABILITY	9
ROBUST SUMMARIES AND CONSTRUCTION OF DATA MATRIX	10
EVALUATION OF MATRIX DATA PATTERNS	10
Evaluation of "Read Across" Patterns	11
Physical-Chemical Properties	11
Environmental Fate and Transport.....	12
Ecotoxicity	13
Toxicity	14
Evaluation of "Read Down" Patterns	15
SUMMARY OF LAB SULFONIC ACIDS CATEGORY PROPERTIES	15
CONCLUSIONS.....	16
REFERENCES	18

LIST OF TABLES

Table 1.	Typical Alkyl Chain Composition
Table 2.	Sponsored LAB Sulfonic Acids
Table 3.	Environmental Distribution of Sponsored LAB Sulfonic Acids
Table 4.	Data Availability and Assessment Plan Status for the Category

LIST OF APPENDICES

Appendix A.	Table A-1: Summary of Data Available for the LAB Sulfonic Acids
Appendix B.	IUCLID Data Set

EXECUTIVE SUMMARY

The Linear Alkylbenzene (LAB) Sulfonic Acids Coalition (Coalition) is sponsoring three linear alkylbenzene sulfonic acid materials. These acids are intermediates in the manufacture of linear alkylbenzene sulfonate (LAS) surfactants, a major cleaning agent in laundry detergents. The Coalition assembled and reviewed the available public and private toxicological data, and developed an assessment plan for the sponsored materials. Because of the close structural similarity between LAS and the LAB sulfonic acids, data from LAS are included to provide supporting information for the category.

The LAB sulfonic acids are highly water soluble (miscible) and have a relatively low K_{ow} . The environmental fate data indicate that these chemicals are highly susceptible to photo- and biodegradation. The acute aquatic toxicity is consistent across the four chemicals for fish, *Daphnia*, and algae. The acute oral mammalian toxicity is similar and of low concern for all of the chemicals with available data. LAS data on the chronic aquatic toxicity, repeated dose, reproductive and developmental endpoints do not indicate any significant areas of concern for the LAB sulfonic acids.

Furthermore, the LAB sulfonic acids are exclusively used as intermediates in the production of LAS. Worker exposure potential is extremely small and highly controlled through the use of engineering controls, personal protective equipment, and use of closed production systems. There is no consumer exposure to LAB sulfonic acids since they are not used in consumer products.

Based on the availability of data and the limited exposure potential, the LAB sulfonic acids are considered to be of low concern and no further testing is necessary for the materials in the category.

INTRODUCTION

The High Production Volume (HPV) Challenge Program is a voluntary initiative of the US chemical industry to complete hazard data profiles for approximately 2800 HPV chemicals as identified on the US Environmental Protection Agency's (USEPA) 1990 Toxic Substances Control Act (TSCA) Inventory Update Rule (IUR). In the US, HPV chemicals are those that are manufactured or imported in quantities greater than 1 million pounds per year. The hazard data to be provided in the program are those that meet the requirements of the Screening Information Data Set (SIDS) Program (OECD 1997). SIDS, which has been internationally agreed to by member countries of the Organization for Economic Cooperation and Development (OECD), provides the basic screening data needed for an initial assessment of the physical-chemical properties, environmental fate, and adverse human and environmental effects of chemicals. The information for completing the SIDS can come from existing data or may be generated as part of the HPV Challenge Program. Once the available studies are identified or conducted, "robust summaries" are prepared.

The USEPA, industry, and non-governmental organizations (NGOs) are unified in their commitment to minimize the numbers of animals tested in the HPV Challenge Program whenever it is scientifically justifiable (USEPA 1999a, 2000a). One approach is to evaluate closely related chemicals as a group, or category, rather than solely as individual chemicals. The use of categories is encouraged by USEPA in the HPV Challenge Program. Appropriately constructed categories allow for a more efficient evaluation while reducing the number of animals required for testing.

The Linear Alkylbenzene (LAB) Sulfonic Acids Coalition (Coalition) has agreed to assemble and review available public and private toxicological data, develop and provide an assessment plan for the sponsored chemicals and conduct additional research, including testing when necessary, for three linear alkylbenzene sulfonic acids. These acids are intermediates in the manufacture of linear alkylbenzene sulfonate surfactants, a major cleaning agent in laundry detergents. The Coalition is comprised of the following member companies:

Colgate-Palmolive Company
Akzo Nobel Surface Chemistry LLC
The Dial Corporation
Stepan Company
Unilever HPC-USA

This assessment plan is the result of the Coalition's efforts and provides a summary and analysis of the available data, and identifies any data gaps in the SIDS data profile. Section II of this assessment plan provides a rationale and justification for the development of the LAB Sulfonic Acid category. Section III reviews the methods used in the collection of published and unpublished data. Section IV reviews the evaluation of data quality. Section V reviews the preparation of the robust summaries and the construction of a data matrix. Section VI is an in-depth evaluation of data matrix patterns for each of the four data endpoint categories (*i.e.*, physical-chemical properties, environmental fate, ecotoxicity and mammalian toxicity). Section VII is a summary of the LAB Sulfonic Acid category and its properties. Section VIII presents the conclusions regarding data availability and identifies data gaps in the SIDS profiles for the sponsored chemicals.

IDENTIFICATION OF STRUCTURE BASED CATEGORY

The LAB Sulfonic Acids Coalition is sponsoring three chemicals from the 1990 and 1994 IURs:

Benzene sulfonic acid, C₁₀₋₁₆ alkyl derivatives (CAS# 68584-22-5),
Benzene sulfonic acid, dodecyl (CAS# 27176-87-0), and,
Benzene sulfonic acid, tridecyl (CAS# 25496-01-9).

Structural, process and use similarities among these substances, evaluation of existing data, and professional judgement were used to define a LAB Sulfonic Acids category for the HPV Challenge Program. The LAB Sulfonic Acids category consists of linear alkylbenzene sulfonic acid homologues with alkyl carbon chain lengths ranging from C₁₀ to C₁₄ and averaging 11.0 to

12.9. The primary structure is a C₁₀ to C₁₄ linear alkyl chain with a *para*-substituted benzene sulfonic acid group attached at any of the secondary alkyl carbon positions.

The LAB sulfonic acids are intermediates in the manufacture of linear alkylbenzene sulfonate (LAS) surfactants, a major cleaning agent for laundry detergents and other cleaning products. The feedstocks for the manufacture of the LAB sulfonic acids are linear alkyl benzenes (LAB). LAB is made by reacting a mixture of C₁₀ to C₁₄ n-paraffins with benzene. The alkyl attachment occurs at all but the terminal carbon positions. Consequently, LAB is a mixture of C₁₀ to C₁₄ linear alkyl chain homologues with average alkyl chain lengths between 11.3 and 12.6 (See Table 1) attached at any of the secondary (non-terminal) positions to the benzene ring.

LAB made in Europe has alkyl chain lengths ranging from C₁₀ to C₁₃ and averaging 11.6 (Valtorta et al, 2000). The alkyl chain distribution of this LAB is shown in Table 1.

Table 1

TYPICAL ALKYL CHAIN COMPOSITION*

US LAB TRADE NAMES	TYPICAL ALKYL CARBON CHAIN COMPOSITION PERCENT OF TOTAL					CALCULATED AVERAGE ALKYL CHAIN LENGTH**
	C ₁₀	C ₁₁	C ₁₂	C ₁₃	C ₁₄	
Alkylate 215	15	40	40	4	<1	11.3
Nalkylene 550L	14	30	29	20	7	11.8
Alkylate 225	9	32	38	20	<1	11.6
Nalkylene 575L	9	17	28	30	15	12.2
Alkylate 229	1.5	7.5	35	46	10	12.6
European LAB***	13-14	29-34	30-32	17-21	<1	11.6
LAS	1-25	7-50	20-50	5-45	<1-10	11.7****

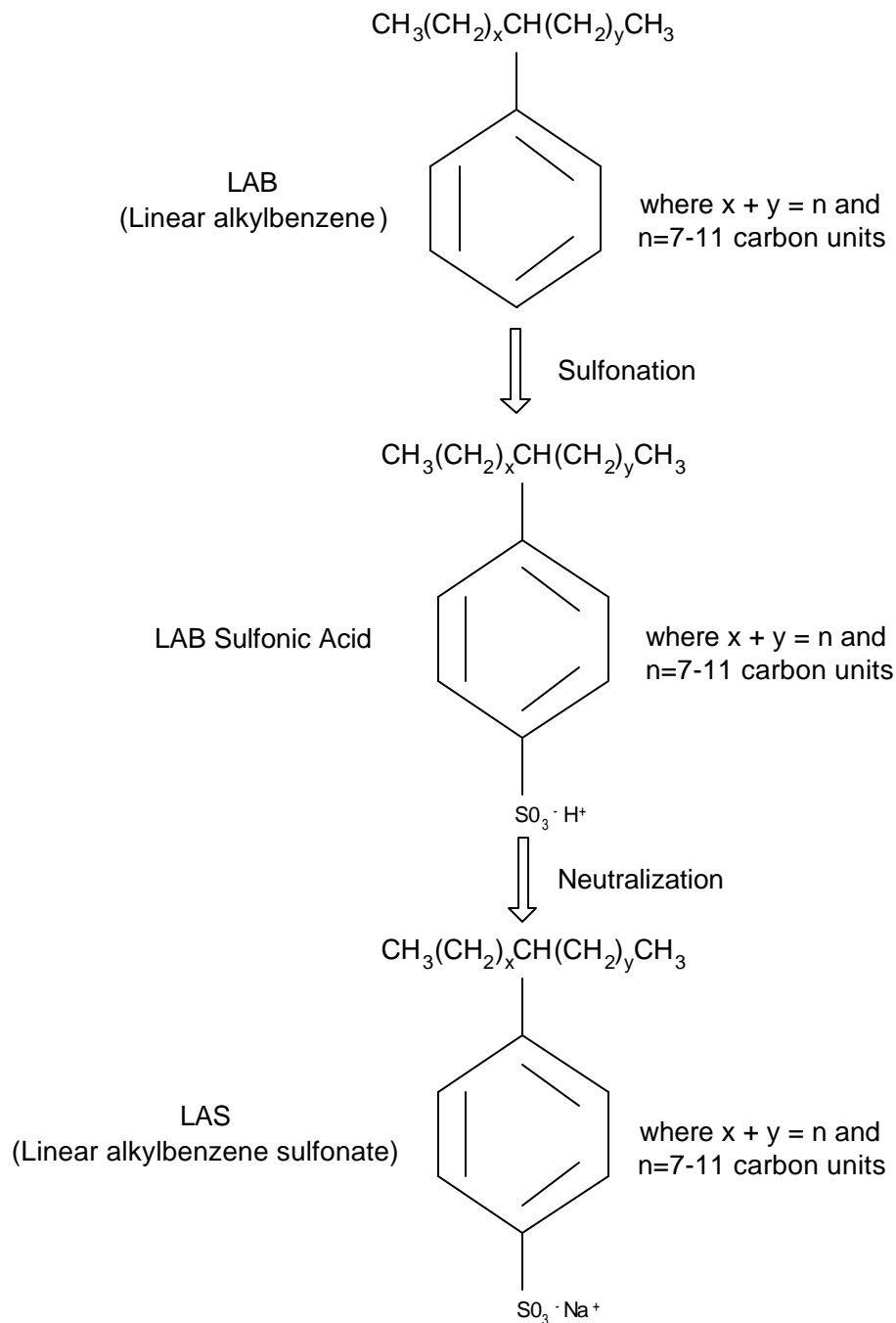
* Source: USEPA. 2002. Updated LAB SIDS report. (SIDS Initial Assessment Report (SIAR), Benzene, C10-16 Alkyl Derivatives, CAS Nos. 123-01-3, etc.)

** Calculated as $(10 \times \%C_{10}/100) + (11 \times \%C_{11}/100) + (12 \times \%C_{12}/100) + (13 \times \%C_{13}/100) + (14 \times \%C_{14}/100)$

*** Source: Valtorta et al. 2000

**** The reported average alkyl chain length for LAS is weighted by United States production volume. Data from the LAS Coalition draft Assessment Plan dated January 9, 2003.

The LAB is then reacted with SO_3 or sulfuric acid to make LAB sulfonic acids. The sulfonate group is *para* to the alkyl chain attachment on the benzene ring. The LAB sulfonic acids are, in turn, neutralized to the sodium salts, LAS. This relationship is shown below. LAB and LAS are being addressed through the SIDS program¹.



¹ An OECD SIDS assessment of LAB was completed in 1995 (the SIAP is available at www1.oecd.org/ehs/sidstable/123013.pdf). The USEPA has completed its review of a SIDS dossier and assessment report for LAS, and the LAS SIDS Consortium is currently preparing the remaining SIDS documents for submission to the USEPA in preparation for SIAM 17 (November 2003).

Although CAS# 68584-22-5 is named benzene sulfonic acid, C₁₀₋₁₆ alkyl derivatives, the proportion of C₁₅ and C₁₆ alkyl chains in LAB is <1%, therefore, C₁₀₋₁₆ LAB sulfonic acids do not contain any significant C₁₅ or C₁₆ constituents. In fact, alkyl chain lengths for the C₁₀₋₁₆ benzene sulfonic acids range from C₁₀ to C₁₄ and average 11.3 to 11.8. The dodecylbenzene sulfonic acids (CAS# 27176-87-0) also are mixtures of C₁₀ to C₁₄ alkyl benzene sulfonic acids with average alkyl chain lengths of 11.3 to 12.6. Similarly, tridecylbenzene sulfonic acids (CAS# 25496-01-9) are mixtures of C₁₀ to C₁₄ alkylbenzene sulfonic acids with average alkyl chain lengths of 11.8 to 12.6. Overall, alkyl chain lengths for US-produced LAB sulfonic acids range from C₁₀ to C₁₄ and average from 11.3 to 12.6. The reported average alkyl chain length for LAS is 11.7, as weighted by United States production volume.

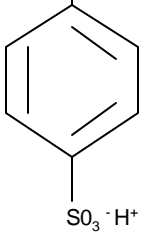
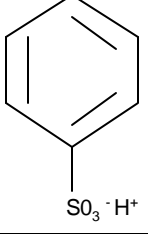
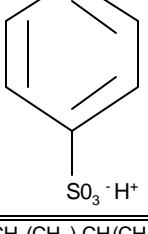
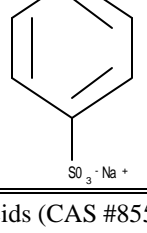
Table 2 presents the sponsored chemicals plus LAS, their CAS numbers, representative structures and average alkyl chain lengths.

Relationship of US to European LAB Sulfonic Acids

European LAB sulfonic acids (CAS # 85536-14-7) have the same alkyl chain distribution as European LAB (See Table 1), with alkyl chain lengths ranging from C₁₀ to C₁₃ and averaging 11.6 (Valtorta et al., 2000). European LAB sulfonic acids have an average alkyl chain distribution (11.6) in the range of those reported for the C₁₀₋₁₆ LAB sulfonic acids (11.3 to 11.8). European LAB sulfonic acids have C₁₄ homologue levels similar to the C₁₀₋₁₆ LAB sulfonic acids (<1 to 7%). Because of the similarity of the alkyl chain distributions of European LAB sulfonic acids to those of the C₁₀₋₁₆ LAB sulfonic acids, data obtained from studies of European LAB sulfonic acids (CAS # 85536-14-7) are applicable to the C₁₀₋₁₆ LAB sulfonic acids (CAS # 68584-22-5).

Table 2

SPONSORED LAB SULFONIC ACIDS

COMPOUND/ MIXTURE	CAS NUMBER	REPRESENTATIVE STRUCTURE	AVERAGE ALKYL CHAIN LENGTH
Benzene sulfonic acid, C ₁₀₋₁₆ alkyl derivatives	68584-22-5	$\text{CH}_3(\text{CH}_2)_x\text{CH}_2(\text{CH}_2)_y\text{CH}_3$  <p>where $x + y = n$ and $n=7-11$ carbon units</p>	11.3-11.8*
Benzene sulfonic acid, dodecyl (C ₁₂)	27176-87-0	$\text{CH}_3(\text{CH}_2)_x\text{CH}_2(\text{CH}_2)_y\text{CH}_3$  <p>where $x + y = n$ and $n=7-11$ carbon units</p>	11.3-12.6
Benzene sulfonic acid, tridecyl (C ₁₃)	25496-01-9	$\text{CH}_3(\text{CH}_2)_x\text{CH}_2(\text{CH}_2)_y\text{CH}_3$  <p>where $x + y = n$ and $n=7-11$ carbon units</p>	11.8-12.6
[Supporting Substance] Linear Alkylbenzene Sulfonate (LAS)	68411-30-3 1322-98-1 25155-30-0 26248-24-8 27636-75-5 68081-81-2 85117-50-6	$\text{CH}_3(\text{CH}_2)_x\text{CH}(\text{CH}_2)_y\text{CH}_3$  <p>where $x + y = n$ and $n=7-11$ carbon units</p>	11.3-12.6

* Range includes European LAB sulfonic acids (CAS #85536-14-7), which have an average alkyl chain length of 11.6.

Relationship of LAB Sulfonic Acids to LAS

The LAB sulfonic acids are strong acids ($pK_a < 1$) that are completely ionized in aqueous solutions (Lide 1990; Noller 1966). The chemical species present in aqueous solutions at neutral (physiological) pH is the LAS ion (C_{10-14} linear alkyl benzene- SO_3^-), the identical species present in solutions of LAS, where the sodium ion will disassociate to form the LAS anion. Thus, the physical-chemical, environmental fate, ecotoxicity and toxicity properties of the LAB sulfonic acids and LAS would be expected to be similar. Therefore, the LAS hazard assessment data already compiled and submitted under the OECD SIDS program can be used as supporting data to supplement any LAB sulfonic acid hazard data to characterize behavior in the environment.

Use Patterns and Exposure Potential

Based on 1998 IUR data, LAB sulfonic acid production in the United States was approximately 100,000, 50,000 and 2,000 tons for CAS numbers 68584-22-5, 27176-87-0, and 25496-01-9, respectively. The carbon chain distributions of the LAB Sulfonic Acids are reflective of the carbon chain distribution of the LAB feedstock ($C_{10}-C_{14}$). The entire production of these LAB sulfonic acids is used as intermediates in the production of LAS. In many, but not all, cases the intermediates are site limited, *i.e.*, they remain on the production facility for use in the LAS production process. In some cases the intermediates are sold to outside LAS manufacturers. Transport to these off-site facilities is conducted following strict health and safety procedures and DOT requirements.

All processing of LAB and LAB sulfonic acids takes place in closed systems that significantly minimize worker exposure. Workers also wear standard personal protective equipment including safety goggles, face shields, safety shoes, impervious nitrile gloves, long sleeved clothing, and rubber boots. Workers may also employ cartridge-type respirators equipped with organic vapor cartridges and acid-resistant suits, for example, during steaming and washing. The closed production process and use of personal protective equipment effectively eliminates exposure to production workers. Un-ionized LAB sulfonic acid is not present after neutralization during manufacture of LAS detergent products. Therefore, no consumer exposure to LAB Sulfonic Acids from detergent use is possible.

Extensive engineering controls are in place to minimize releases to the environment. These controls include SO_2/SO_3 monitoring devices, spill containment dikes for rail unloading, leak inspections, high level tank alarms, and auto shut off valves. Emissions controls include line cyclones, electrostatic precipitation and passing through caustic scrubbers and scrubbing demisters. Some process wastewater is deep well injected. These practices and controls effectively reduce LAB sulfonic acid releases to the environment to levels far below the allowable amounts, as shown by process stack monitoring.

Based on the use patterns described above, no significant exposure to LAB sulfonic acids will occur for workers, consumers, or the environment.

COLLECTION OF UNPUBLISHED AND PUBLISHED DATA

Coalition member companies contributed in-house studies of physical-chemical properties, environmental fate and transport, ecotoxicity, and mammalian toxicity for the chemicals and mixtures in the category. To supplement the industry data, literature searches were conducted of on-line databases (*e.g.*, Hazardous Substances Databank [HSDB], Registry of Toxic Effects of Chemical Substances [RTECS], and Aquatic Toxicity Information Retrieval [AQUIRE]), standard scientific data compendia (*e.g.*, *CRC Handbook of Chemistry and Physics* and *The Merck Index*), and other published sources (*e.g.*, International Uniform Chemical Information Database [IUCLID]). The sum total of the in-house studies, reference books, and literature searches of on-line databases was the identification of a substantial amount of available data for the sponsored chemicals, which are supplemented by the data for the structurally similar LAS.

EVALUATION OF DATA FOR QUALITY AND ACCEPTABILITY

The collected data were reviewed for quality and acceptability following the general USEPA and OECD SIDS guidance (USEPA 1999b; OECD 1997) and the systematic approach described by Klimisch et al. (1997). These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. The Klimisch et al. (1997) approach specifies four categories of reliability for describing data adequacy. These are:

1. **Reliable without Restriction:** Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.
2. **Reliable with Restrictions:** Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.
3. **Not Reliable:** Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.
4. **Not Assignable:** Includes studies or data in which insufficient detail is reported to assign a rating, *e.g.*, listed in abstracts or secondary literature.

Only those studies which are deemed reliable for the current HPV Challenge Program purposes are included in the data set for this assessment plan. Reliable studies include both categories rated 1 (Reliable without restriction) and 2 (Reliable with restrictions). Studies rated 3 (Not reliable) were not used. Studies rated 4 (Not assignable) were used when professional judgment deemed it appropriate as part of a weight-of-evidence approach. Finally, some older studies were not included if they had been superseded by more recent studies rated 1.

Much of the available data were from study reports conducted by either outside contract laboratories or in-house industry laboratories. These study reports followed standard procedures for testing of physical-chemical properties, environmental fate and transport, aquatic toxicity, and mammalian toxicity. Some of the most recent studies were conducted under GLP provisions. In addition, some data were obtained from the published, peer-reviewed, scientific literature. Reliable data from all of these sources were incorporated into the data set as appropriate. Overall, a substantial amount of data of high quality were available for chemicals and mixtures in the LAB Sulfonic Acid category.

ROBUST SUMMARIES AND CONSTRUCTION OF DATA MATRIX

Robust summaries were prepared according to the format recommended by the USEPA (1999c) and OECD (1997) and entered into the standard International Uniform Chemical Information Database (IUCLID) software. These summaries present the salient information from each of the reliable studies. All of the summaries are collected into a dossier that includes all of the individual chemicals and mixtures for the category. The robust summary dossier for the LAB Sulfonic Acid category is attached as an appendix and should be used in conjunction with this assessment plan.

Table A-1 in the Appendix to this assessment plan is a matrix of SIDS/HPV endpoints and the available data for each of the sponsored chemicals in the LAB Sulfonic Acid category. In addition, the table includes data for LAS, which support the overall predictive value of the category. Data drawn from the robust summaries are shown in the table for each endpoint and chemical when available. The data presented for LAS were derived from a dossier being developed for the OECD SIDS program and include a total of seven CAS numbers, all representative of LAS.

EVALUATION OF MATRIX DATA PATTERNS

Table A-1 identifies where data for specific compounds and data endpoints are available (data provided) and not available (indicated by "--" in the table). The available data were evaluated for patterns and trends related to structure that then could be used to predict values for a particular endpoint (*e.g.*, acute oral toxicity) where adequate data are not available (*i.e.*, "Read Across"). In addition, the data were evaluated to determine to what extent the SIDS data endpoints were covered by available data for each chemical (*e.g.*, dodecylbenzene sulfonic acid) in the category (*i.e.*, "Read Down").

Evaluation of "Read Across" Patterns

The following discussion reviews the "read across" patterns identified for each of the four major data areas: physical-chemical properties, environmental fate and transport, ecotoxicity, and mammalian toxicity.

Physical-Chemical Properties

The primary patterns in the physical-chemical properties of chemicals in the LAB Sulfonic Acids category are trends in the parameters that affect partitioning between air and water, and between water and organic phases (*e.g.*, soil or biota). The most important of these parameters are vapor pressure, water solubility, and the octanol/water partition coefficient (K_{ow}). Because of the narrow range of carbon chain lengths covered by the category, it would be expected that their physical-chemical properties would be similar.

It should be noted that the LAB sulfonic acids are liquids and LAS is a solid at room temperature. Thus, certain physical-chemical parameters are not appropriate to compare (*e.g.*, melting and boiling points). However, in water the difference between the LAB sulfonic acids and LAS disappears as dissociation results in the same ion in solution. Therefore, parameters such as K_{ow} , water solubility and pH/ pK_a are appropriate to compare.

Melting and boiling point data are available for two of the LAB sulfonic acids. The IUCLID data sheet for benzene sulfonic acid, C₁₀₋₁₆-alkyl derivatives (CAS #68584-22-5) cites a Shell Chemicals report indicating a melting point of $-10\text{ }^{\circ}\text{C}$, consistent with materials that are liquids at room temperature. A CONDEA Vista material safety data sheet reports the same melting point value for an alkylbenzene sulfonic acid mixture. The IUCLID data sheet for dodecylbenzene sulfonic acid (CAS #27176-87-0) cites a Hoechst Iberica s.a. report with a melting point also of $-10\text{ }^{\circ}\text{C}$, while a standard reference compilation (Verschuere 1996) reports a melting point of $10\text{ }^{\circ}\text{C}$ ². Boiling point data for the CONDEA Vista alkylbenzene sulfonic acid mixture indicate a value of $156\text{ }^{\circ}\text{C}$. The IUCLID data sheet for dodecylbenzene sulfonic acid (CAS #27176-87-0) cites a Hoechst Iberica s.a. report with a boiling point $205\text{ }^{\circ}\text{C}$, while Verschuere reports a value of $315\text{ }^{\circ}\text{C}$ for this chemical.

The only vapour pressure information is a value of 0.22 hPa for the CONDEA Vista alkylbenzene sulfonic acid mixture. However, LAB sulfonic acids are not expected to volatilize significantly, as noted in the fugacity discussion below.

The octanol-water partition coefficients are around 2 ($\log K_{ow}$) for all of the chemicals in this category. A Shell Chemical report cited in the IUCLID for benzene sulfonic acid, C₁₀₋₁₆-alkyl derivatives (CAS #68584-22-5) indicates a measured K_{ow} value of 2 using the

² Given the other available results, it is likely that this is a typographical error in the text and the actual value is $-10\text{ }^{\circ}\text{C}$.

Shake-Flask method. The other values are estimated using the Leo and Hansch formula and show good agreement with the measured value. Similarly, the available data indicate that all of the chemicals are very highly soluble in water, with reported values of up to 400,000 mg/L (40%).

No further testing is necessary because of the similarities between the sulfonic acids and LAS in solution.

Environmental Fate and Transport

The important information from the environmental fate data is the primary mechanism or mechanisms of degradation and whether there is any pattern to differences observed between chemicals. For organic chemicals, this is commonly the breakdown of compounds into smaller constituents by biological degradation. Other breakdown mechanisms that may be important are photolysis and hydrolysis. These breakdown mechanisms are necessarily dependent on what environmental compartment (air, water, soil, sediment) to which the chemicals are distributed. Fugacity modeling can be used to estimate the relative percentage of chemicals that will partition to various compartments at steady state. The results of the modeling using the EPI Suite of estimation programs (USEPA 2000b) are shown in Table 3.

Table 3

ENVIRONMENTAL DISTRIBUTION OF SPONSORED LAB SULFONIC ACIDS BASED ON EQC MODELING

Environmental Compartment	Benzene sulfonic acid, C10-16 alkyl derivatives*	Benzene sulfonic acid, dodecyl-	Benzene sulfonic acid, tridecyl-	[Supporting Substance] Linear Alkylbenzene Sulfonate (LAS)*
Air	1%	<1%	<1%	1%
Water	32%	29%	23%	34%
Soil	63%	60%	53%	65%
Sediment	4%	10	23%	<1%

* A C₁₁ benzene sulfonic acid alkyl derivative and a C₁₂ LAS were modeled for the benzene sulfonic acid, C₁₀₋₁₆ alkyl derivatives and LAS, respectively because these chain lengths more closely match the average alkyl chain lengths of these materials. The model assumes a C₁₂ and C₁₃ alkyl chain length for the dodecyl- and tridecyl-benzene sulfonic acids, respectively. See the corresponding robust summaries for further details.

Based on physical-chemical properties, the fugacity modeling predicts that most of the sponsored chemicals will partition to the soil and water. Very little partitions to the air or sediment.

The atmospheric oxidation potential of the three sponsored chemicals in the category was estimated using the EPI Suite software (v. 3.10; USEPA 2000b). These estimations suggest that photodegradation may be a significant mechanism for the breakdown of

benzene sulfonic acids. Based on the model estimates, the hydroxyl radical reaction half-lives ranged from about 7 to 8.6 hours. Estimated data for LAS were similar. Furthermore, measured data for LAS suggest even more rapid photodegradation, with 95% of the material degraded within 20 minutes at 20 °C in a laboratory study. With respect to stability in water, no hydrolysis information is available for the three sulfonic acids, but data do indicate that LAS is stable in water.

Measured biodegradation data are available for two of the sponsored chemicals in the category and LAS. These data indicate substantial microbial degradation under aerobic conditions. For dodecylbenzene sulfonic acid, the one available study indicates 69% of the material mineralized after 28 days³. Biodegradation of the C₁₀₋₁₆ derivatives and the LAS are also rapid, with 93% or greater of the material degrading within 28 or 37 days. In addition, studies show that straight chain alkylbenzene sulfonate materials readily degrade, with the shorter chain length compounds degrading more rapidly (Eden et al. 1968).

Thus, the data indicate that these chemicals are highly susceptible to degradation, both by photolytic and microbial mechanisms. Available data also indicate that they have low to moderate bioaccumulation potential, with a bioconcentration factor for dodecyl benzene sulfonic acid of 130. LAS has bioconcentration factors that range from 22 to 87. No additional environmental fate studies are necessary to characterize these materials.

Ecotoxicity

The primary pattern from ecotoxicity is whether the toxicity to aquatic organisms changes predictably with structural differences in the materials. In addition, it is important to evaluate whether the physical-chemical properties of the chemicals affect their bioavailability, and subsequently, their aquatic toxicity.

Acute fish toxicity data are available for all three of the sponsored chemicals in the category and LAS. The data indicate very similar toxicity levels of these chemicals to fish, with LC₅₀ values range from about 3 to 6 mg/L. Data are also available for toxicity to the invertebrate *Daphnia magna* for all four chemicals. These data similarly show a very narrow range in toxicity values, with EC₅₀ values falling into a range between about 3 to 12 mg/L. Finally, data on the toxicity of three of the four chemicals to algae are also available. These data show EC₅₀ values in a range from 29 to 170 mg/L. Given the complete coverage of the aquatic acute toxicity across species and the narrow ranges in results, no additional acute ecotoxicity testing is necessary. Chronic aquatic toxicity data are not required for the HPV Challenge Program. However, chronic data are available for LAS, and given that the sulfonic acids in aqueous solutions produce the identical ion as LAS, no further chronic toxicity testing is necessary.

³ Mineralization refers to the complete degradation of the chemical to CO₂ and water. Biodegradation refers to degradation of the parent chemical into other materials, but does not necessarily include complete mineralization to CO₂ and water.

Toxicity

Toxicity to mammals is an important surrogate for estimating potential affects on humans. Again, patterns are evaluated to determine if data endpoints without values can be estimated from the data that are available. Several aspects of mammalian toxicity are evaluated. Acute testing provides information on gross effects, such as mortality, from exposure to high doses. Repeated dose testing provides information on toxicity associated with multiple doses over time. Genetic testing is conducted to evaluate the potential for mutagenic effects by using bacterial systems (*e.g.*, the Ames test), non-bacterial systems (*e.g.*, cell transformation), and in vivo (*i.e.*, live animal) systems. Reproductive and developmental/teratogenic testing provides information on the potential effects of long-term exposure to lower doses, especially as related to possible effects in developing embryos and young animals. It is important to note that the lack of significant exposure may obviate the need to fill apparent data gaps with mammalian testing.

There are three primary routes of exposure used in the evaluation of acute toxicity: 1) oral, where the test substance is introduced in food or directly into the test animal by gavage; 2) inhalation, where the substance is introduced into the lungs; and 3) dermal, where the substance is applied directly to the skin. The choice of exposure route depends on the physical-chemical characteristics of the test substance and the likely route by which animals or humans would be exposed. Data for all three routes of exposure are usually not necessary to understand the acute toxicity of a particular chemical substance.

For the LAB Sulfonic Acids category, acute oral toxicity data are available for two of the three sponsored sulfonic acids and LAS. The data indicate minimal to moderate toxicity, with LD₅₀ values ranging from 500 to 2000 mg/kg body weight (bw). Acute inhalation data are available for LAS only, and indicate a lack of significant toxicity. Dermal exposure data are available for one of the LAB sulfonic acids and also indicates a lack of significant toxicity. In vitro bacterial and in vivo genetic toxicity studies are available for the C₁₀₋₁₆ alkyl derivatives (CAS #68584-22-5) and these endpoints plus an in vitro non-bacterial genetic toxicity study are available for LAS. All of these studies proved negative for mutagenicity. Data on repeated dose exposures, reproductive toxicity, and developmental toxicity/teratogenicity are available for LAS and indicate a lack of significant effects on these endpoints. The data indicate that LAS is of low concern.

Besides the SIDS endpoints, data are provided on several “Beyond-SIDS” endpoints for completeness. These are endpoints that are not required by the HPV Chemical Challenge Program but are available and offer additional insight to the health and safety of the materials. For example, skin and eye irritation and sensitization potential studies are available for two of the sponsored materials and LAS. Results show that these materials can be irritating if in contact with the skin or eyes, but they were not dermally sensitizing. Carcinogenicity data for LAS indicate no differences in tumor incidence in rats with oral feed exposure for two years.

Overall, the mammalian toxicity of LAB Sulfonic Acids has been well characterized, especially when the data for LAS are considered. Results indicate a lack of significant mammalian toxicity. Data for repeated dose exposures, and reproductive and developmental endpoints are lacking for the three sponsored chemicals, but are available for LAS. Given the close relationship between LAS and the LAB Sulfonic acids, these data should suffice. In addition, the sole use of LAB sulfonic acids as intermediates in the production of LAS virtually eliminates the possibility for long-term consumer exposures. Potential occupational exposures are mitigated by the use of closed production systems and personal protective equipment. Therefore, no additional toxicity testing is deemed necessary to characterize the toxicity of the LAB Sulfonic Acids category.

Evaluation of “Read Down” Patterns

Data are available for each of the individual chemicals in the category. A complete data set is available for LAS, and, with the exception of chronic aquatic toxicity and mammalian toxicity, complete data sets are available for the three LAB Sulfonic acids. For mammalian toxicity, oral toxicity data are available for two of the three sponsored chemicals and the results are similar to the results for LAS. It is important to note that all of the LAB Sulfonic Acids are intermediates in the manufacture of LAS and LAS-related materials. Therefore there is extremely limited environmental, occupational, and commercial exposure potential. Given this limited exposure, the similarity in physical-chemical, environmental fate, ecotoxicity and toxicity data, as well as the complete data set for LAS, no additional testing is warranted.

SUMMARY OF LAB SULFONIC ACIDS CATEGORY PROPERTIES

The three sponsored chemicals are linear alkylbenzene sulfonic acids representing a range of alkyl chain lengths (C₁₀-C₁₄). They are intermediates in the manufacture of LAS, and comprise the LAB Sulfonic Acids category. Because of the close structural similarity between LAS and the LAB sulfonic acids, data from LAS are included to provide supporting information for the category. All of the relevant physical-chemical properties are similar between the chemicals. They are highly water soluble (miscible) and have a relatively low K_{ow}.

The environmental fate data indicate that these chemicals are highly susceptible to photo- and biodegradation. The acute aquatic toxicity is consistent across the four chemicals for fish, *Daphnia*, and algae. Similarly, acute oral mammalian toxicity is similar and of low concern for all of the chemicals with available data. LAS data on the chronic aquatic toxicity, repeated dose, reproductive and developmental endpoints do not indicate any significant areas of concern.

Table 4 shows the availability of data and assessment plan status for the LAB Sulfonic Acids category.

CONCLUSIONS

Substantial data are available for the three sponsored LAB sulfonic acids and LAS, the supporting substance. These data show consistent results across the LAB sulfonic acids category and are generally not a toxicological concern. Furthermore, the LAB sulfonic acids are exclusively used as intermediates in the production of LAS. Worker exposure is extremely limited and highly controlled through the use of engineering controls, personal protective equipment, and use of closed production systems. There is no consumer exposure to LAB sulfonic acids since they are not used in consumer products.

Based on the availability of data and the limited exposure potential, the LAB sulfonic acids are considered to be of low concern and no further testing is necessary for the materials in the category.

Table 4

**DATA AVAILABILITY AND ASSESSMENT PLAN STATUS FOR THE LAB
SULFONIC ACID CATEGORY**

	Data Available	Data Acceptable	Testing Required
Physical-Chemical Properties			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
Octanol/Water Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	N
pH Value, pK _a Value	Y	Y	N
Environmental Fate and Pathways			
Photodegradation	Y	Y	N
Stability in Water	Y *	Y	N
Biodegradation	Y	Y	N
Bioaccumulation	Y	Y	N
Ecotoxicity			
Acute/Prolonged Toxicity to Fish	Y	Y	N
Acute Toxicity to <i>Daphnia</i>	Y	Y	N
Toxicity to Aquatic Plants (algae)	Y	Y	N
Chronic Toxicity to Fish	Y *	Y	N
Chronic Toxicity to Aquatic Invertebrates	Y *	Y	N
Toxicity			
Acute Oral Toxicity	Y	Y	N
Acute Inhalation Toxicity	Y *	Y	N
Acute Dermal Toxicity	Y	Y	N
Skin Irritation	Y	Y	N
Eye Irritation	Y	Y	N
Skin Sensitization	Y	Y	N
Repeated Dose Toxicity	Y *	Y	N
Genetic Toxicity in vitro (Bacterial test)	Y	Y	N
Genetic Toxicity in vitro (Non- bacterial test)	Y *	Y	N
Genetic Toxicity in vivo	Y	Y	N
Carcinogenicity	Y *	Y	N
Toxicity to Reproduction	Y *	Y	N
Developmental Toxicity	Y *	Y	N

* Surrogate data available for the supporting substance Linear Alkylbenzene Sulfonate (LAS)

REFERENCES

- Eden, G.E., Truesdale, G.A., and Stennett, G.V. 1968. Assessment of bioavailability. *Wat. Pollut. Control.* pp.107-123.
- Klimisch, H.-J., Andreae, M., and Tillmann, U. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. *Regul. Toxicol. Pharmacol.* 25:1-5.
- Lide, D.R. 1990. Handbook of Chemistry and Physics. 71st Edition. Ann Arbor: CRC Press.
- Noller, C.R. 1966. Textbook of Organic Chemistry. Third Edition. Philadelphia: W.B. Saunders Company.
- OECD. 1997. SIDS Manual (third revision). Organization for Economic Cooperation and Development. July 1997.
- USEPA. 1999a. HPV Chemical Human Health Testing: Animal Welfare Issues and Approaches. Guidance document dated February 1999.
- USEPA. 1999b. Determining the Adequacy of Existing Data. Draft guidance document dated February 10, 1999.
- USEPA. 1999c. Draft Guidance on Developing Robust Summaries. October 22, 1999.
- USEPA. 2000a. Chemical Right to Know High Production Volume Challenge Program: Fact Sheet on Animal Welfare. July 2000. EPA 745-F-99-003.
- USEPA. 2000b. EPI Suite Estimation Software, v. 3.10.
- Valtorta, L., Radici, P., Calcinai, D., and Cavalli, L. 2000. Recent development of LAB/LAS. *La Rivista Italiana Delle Sostanze Grasse* 77:73-76.
- Verschueren, K. 1996. Handbook of Environmental Data on Organic Chemicals. Third Edition. New York: John Wiley & Sons, Inc.

Table A-1

Summary of Data Available for the LAB Sulfonic Acids

Section	Description	Benzene sulfonic acid, C10-16-alkyl derivatives	Benzene sulfonic acid, dodecyl-	Benzene sulfonic acid, tridecyl-	[Supporting Substance] Linear Alkylbenzene Sulfonate (LAS)
	CAS Number	68584-22-5	27176-87-0	25496-01-9	68411-30-3 et al.
	Physical-Chemical Data				
2.1	Melting Point	<-10°C	10°C	--	198.5°C
2.2	Boiling Point	156°C	315°C, 205°C	--	Decomposition onset at 444°C
2.4	Vapour Pressure	0.22 hPa	--	--	3 x 10 ⁻¹³ Pa
2.5	Octanol/Water Partition Coefficient (log)	2.0 at 23°C	1.96	2.52	3.32
2.6.1	Water Solubility	Miscible up to 40% (4 x 10 ⁵ mg/L at 20°C)	3 x 10 ⁵ mg/L at 20°C	--	2.5 x 10 ⁵ mg/L at 20°C
	pH Value, pKa Value	pKa < 1	pKa < 1	pKa < 1	pH = 10 (1% solution)
	Environmental Fate and Pathways				
3.1.1	Photodegradation	t _{1/2} = 8.6 hrs	t _{1/2} = 7.9 hrs	t _{1/2} = 7.2 hrs	>95% after 20 minutes
3.1.2	Stability in Water	--	--	--	stable
3.5	Biodegradation	94% biodegradation after 28 days* 92% biodegradation after 37 days*	69% mineralization after 28 days	--	93% after 28 days
3.7	Bioaccumulation	--	3-day BCF(fish) = 130	--	BCF = 22-87
	Ecotoxicity				
4.1	Acute/Prolonged Toxicity to Fish	96-h LC ₅₀ =5.6 mg/L*	96-h LC ₅₀ =4.1, 10, 4.3 mg/L	96-h LC ₅₀ =3 mg/L	96-h LC ₅₀ = 5.8 mg/L LC ₅₀ = 3.0-3.2 mg/L
4.2 A	Acute Toxicity to Daphnia	48-h EC ₅₀ =5.2 mg/L* 48-h EC ₅₀ =9.3-11.6 mg/L 48-h EC ₅₀ =2.9 mg/L	EC ₅₀ =12, 5.88 mg/L	48-h EC ₅₀ =4.3 mg/L	48-h EC ₅₀ = 6.8 mg/L EC ₅₀ = 4.1-4.7 mg/L
4.3	Toxicity to Aquatic Plants (e.g., algae)	72-h EC ₅₀ =36 mg/L* EC ₅₀ =170 mg/L	EC ₅₀ =50, 29 mg/L		72-h EC ₅₀ = 163 mg/L IC ₅₀ = 9.1 mg/L
4.5.1	Chronic Toxicity to Fish	--	--	--	NOEC = 0.25-3.2 mg/L
4.5.2	Chronic Toxicity to Aquatic Invertebrates	--	--	--	NOEC = 1.4 mg/L
	Toxicity				
5.1.1	Acute Oral Toxicity	LD ₅₀ (rat) = 1,470 mg/kg bw* LD ₅₀ (rat) = 775 mg/kg bw	LD ₅₀ (rat) = 500-2,000 mg/kg bw	--	LD ₅₀ (rat) = 1,080-1,980 mg/kg bw
5.1.2	Acute Inhalation Toxicity	--	--	--	LC ₅₀ = 310 mg/m ³ particulate
5.1.3	Acute Dermal Toxicity	LD ₅₀ (rabbit) = 2,000 mg/kg bw	--	--	LD ₅₀ (rat, rabbit) >2000 mg/kg bw
5.2.1	Skin Irritation	irritating at 0.5 mL*	irritating at 0.5 mL	--	irritating
5.2.2	Eye Irritation	irritating at 0.1 mL*	--	--	irritating
5.3	Sensitization	no sensitizing potential	--	--	not sensitizing
5.4	Repeated Dose Toxicity	--	--	--	NOAEL (rat) = 85 mg/kg bw
5.5	Genetic Toxicity <i>in vitro</i> (Bacterial test)	non-genotoxic	--	--	non-genotoxic
5.5	Genetic Toxicity <i>in vitro</i> (Non-bacterial test)	--	--	--	non-genotoxic
5.6	Genetic Toxicity <i>in vivo</i>	non-genotoxic*	--	--	non-genotoxic
5.7	Carcinogenicity	--	--	--	NOAEL (rat) = 250 mg/kg bw d
5.8	Toxicity to Reproduction	--	--	--	NOAEL (rat) = 350 mg/kg bw d
5.9	Developmental Toxicity/Teratogenicity	--	--	--	NOAEL (rat, oral) = 780 mg/kg bw d NOAEL (mouse, dermal) = 1500 mg/kg bw d

-- No data available

bw = body weight

* Data from European LAB sulfonic acid (CAS #85536-14-7) used as a surrogate.

I U C L I D

D A T A S E T

Existing Chemicals Linear Alkylbenzene (LAB) Sulfonic Acids (LABSA)

Producer

Company: The LAB Sulfonic Acids Coalition

Creation date: December 5, 2000

Prepared by

Company: THE WEINBERG GROUP INC.

Printing date: March 27, 2003

Revision date:

Date of last update: March 27, 2003

Number of pages: 55

I U C L I D

Data Set

Existing Chemical Substance ID: LABSA

Producer Related Part

Company: The Weinberg Group Inc.
Creation date: 05-DEC-2000

Substance Related Part

Company: The Weinberg Group Inc.
Creation date: 05-DEC-2000

Printing date: 27-MAR-2003

Revision date:

Date of last Update: 27-MAR-2003

Number of Pages: 55

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7

Reliability (profile): Reliability: without reliability, 1, 2, 3, 4

Flags (profile): Flags: without flag, confidential, non confidential, WGK
(DE), TA-Luft (DE), Material Safety Dataset, Risk
Assessment, Directive 67/548/EEC

1.0.1 OECD and Company Information

Name: The LAB Sulfonic Acids Coalition

Remark: The Coalition consists of:

Colgate - Palmolive Company
Akzo Nobel Surface Chemistry LLC
The Dial Corporation
Stepan Company
Unilever HPC-USA

21-MAR-2003

1.0.2 Location of Production Site

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.0.3 Identity of Recipients

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.1 General Substance Information

Substance type: organic
Physical status: liquid
Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (CAS# 68584-22-5)
Benzene sulfonic acid, dodecyl- (CAS# 27176-87-0)
Benzene sulfonic acid, tridecyl- (CAS# 25496-01-9)

21-JAN-2002

1.1.1 Spectra

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.2 Synonyms

Lauryl benzene sulfonic acid
29-JUN-2001

Alkylbenzene sulfonic acid
29-JUN-2001

Benzenesulfonic acid, C10-13-alkyl derivatives (CAS# 85536-14-7) [See assessment report for a discussion of the similarity between this European material and Benzene sulfonic acid, C10-16-alkyl derivatives (CAS# 68584-22-5)]
21-JAN-2002

Dodecyl benzene sulfonic acid
29-JUN-2001

Tridecyl benzene sulfonic acid
29-JUN-2001

1.3 Impurities

CAS-No:
EINECS-No:
EINECS-Name:
Remark: None
02-NOV-2001

1.4 Additives

CAS-No:
EINECS-No:
EINECS-Name:
Remark: None
02-NOV-2001

1.5 Quantity

Quantity 100 000 - 500 000 tonnes
05-NOV-2001

1.6.1 Labelling

Labelling:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.6.2 Classification

Classification:
Class of danger:
R-Phrases:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.7 Use Pattern

Type:

Category:

Remark: Primarily as an intermediate in the production of LAS.
02-NOV-2001

1.7.1 Technology Production/Use

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.8 Occupational Exposure Limit Values

Type of limit:

Limit value:

Remark: No TLV has been established
02-NOV-2001

1.9 Source of Exposure

Memo: No significant exposure. See discussion in accompanying LAB
sulfonic acid assessment plan.
02-NOV-2001

1.10.1 Recommendations/Precautionary Measures

Remark: See LAB sulfonic acid assessment plan.
02-NOV-2001

1.10.2 Emergency Measures

Remark: See LAB sulfonic acid assessment plan.
02-NOV-2001

1.11 Packaging

Memo: Bulk transport
02-NOV-2001

1.12 Possib. of Rendering Subst. Harmless

Type of
destruction:

Remark: Not applicable
02-NOV-2001

1.13 Statements Concerning Waste

Memo: See LAB sulfonic acid assessment plan.
02-NOV-2001

1.14.1 Water Pollution

Classified by:
Labelled by:
Class of danger:
Remark: Not a significant source of water pollution.
02-NOV-2001

1.14.2 Major Accident Hazards

Legislation:
Substance listed:
Remark: None
02-NOV-2001

1.14.3 Air Pollution

Classified by:
Labelled by:
Number:
Class of danger:
Remark: Not a significant source of air pollution.
02-NOV-2001

1.15 Additional Remarks

Memo: None
02-NOV-2001

1.16 Last Literature Search

Date of Search: 31-MAY-2001
02-JUL-2001

1.17 Reviews

Memo: None
02-NOV-2001

1.18 Listings e.g. Chemical Inventories

Remark: TSCA inventory (USA)
Domestic Substances List (DSL) - Canada
EINECS (Europe)
21-JAN-2002

2.1 Melting Point

Value: = -10 degree C
GLP: no
Remark: IUCLID cites source as Shell Chemicals U.K. Ltd. Chester
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Reliability: (2) valid with restrictions
21-FEB-2003 (27)

Value: < -10 degree C
GLP: no
Source: CONDEA Vista 1995.
Test substance: Alkylbenzene sulfonic acid with the following composition:

Components	CAS Number	Weight%
Nonylbenzenesulfonic Acid	35298-13-6	0.6
n-Decylbenzenesulfonic Acid	140-60-3	18.3
Undecylbenzenesulfonic Acid	50854-94-9	42.1
Dodecylbenzenesulfonic Acid	27176-87-0	30.0
Tridecylbenzenesulfonic Acid	25496-01-9	4.4
Tetradecylbenzenesulfonic Acid	30776-59-1	0.5
Sulfuric Acid	7664-93-9	1.3
Free Oil	None	2.4
Water	7732-18-5	0.4

Reliability: (4) not assignable
Data from Material Safety Data Sheet. No report available for review.
21-FEB-2003 (4)

Value: = 10 degree C
GLP: no data
Remark: Report not available but based on other sources this may actually be -10 degrees Celcius.
Source: Verschueren 1996.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
Peer-reviewed reference book.
21-FEB-2003 (80)

Value: = -10 degree C
GLP: no data
Remark: IUCLID cites source as Hoechst Iberica s.a. Barcelona.
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
21-FEB-2003 (28)

Value: = 198.5 degree C
Decomposition: yes
Method: other: Thermal analysis was performed on the Netzsch DSC 204C and TG209C with N2 atmosphere.
GLP: no
Remark: This measured melting point value is significantly lower than the EPI Suite estimated values for other LAS materials.

Source: Decomposition onset at 444°C (47% weight loss at 500°C) Huntsman 2002.
Test substance: C10-14 Monoalkylbenzene sulfonic acid, sodium salt (CAS #85117-50-6); mean molecular weight = 348, average alkyl chain length = C12.0. The test material is 85% active matter and is a coarse, cream-colored powder at 25°C.
Reliability: (2) valid with restrictions
21-FEB-2003 (23)

2.2 Boiling Point

Value: = 156 degree C
GLP: no
Source: CONDEA Vista 1995.
Test substance: Alkylbenzene sulfonic acid with the following composition:

Components	CAS Number	Weight%
Nonylbenzenesulfonic Acid	35298-13-6	0.6
n-Decylbenzenesulfonic Acid	140-60-3	18.3
Undecylbenzenesulfonic Acid	50854-94-9	42.1
Dodecylbenzenesulfonic Acid	27176-87-0	30.0
Tridecylbenzenesulfonic Acid	25496-01-9	4.4
Tetradecylbenzenesulfonic Acid	30776-59-1	0.5
Sulfuric Acid	7664-93-9	1.3
Free Oil	None	2.4
Water	7732-18-5	0.4

Reliability: (4) not assignable
Data from Material Safety Data Sheet. No report available for review.
21-FEB-2003 (4)

Value: = 315 degree C
GLP: no data
Source: Verschuere 1996.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
Peer-reviewed reference book.
21-FEB-2003 (80)

Value: = 205 degree C at 1013 hPa
Decomposition: no
GLP: no data
Remark: IUCLID cites source as Hoecht Iberica s.a. Barcelona.
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
21-FEB-2003 (28)

Value:
Decomposition: yes
Method: other: Thermal analysis was performed on the Netzsch DSC 204C and TG209C with N2 atmosphere.
GLP: no
Remark: Decomposition onset at 444°C (47% weight loss at 500°C)
Source: Huntsman 2002.
Test substance: C10-14 monoalkylbenzene sulfonic acid, sodium salt (CAS #85117-50-6); mean molecular weight = 348, average alkyl chain length = C12.0. The test material is 85% active matter and is a coarse, cream-colored powder at 25°C.
Reliability: (2) valid with restrictions
21-FEB-2003 (23)

2.3 Density

Type:
Value:
Remark: Not an HPV Challenge endpoint.
21-MAR-2003

2.3.1 Granulometry

**Type of
distribution:**

Remark: Not an HPV Challenge endpoint.
21-MAR-2003

2.4 Vapour Pressure

Value: = .22 hPa
GLP: no
Source: CONDEA Vista 1995.
Test substance: Alkylbenzene sulfonic acid with the following composition:

Components	CAS Number	Weight%
Nonylbenzenesulfonic Acid	35298-13-6	0.6
n-Decylbenzenesulfonic Acid	140-60-3	18.3
Undecylbenzenesulfonic Acid	50854-94-9	42.1
Dodecylbenzenesulfonic Acid	27176-87-0	30.0
Tridecylbenzenesulfonic Acid	25496-01-9	4.4
Tetradecylbenzenesulfonic Acid	30776-59-1	0.5
Sulfuric Acid	7664-93-9	1.3
Free Oil	None	2.4
Water	7732-18-5	0.4

Reliability: (4) not assignable
Data from Material Safety Data Sheet. No report available for review.

21-FEB-2003 (4)

Value: = 0 hPa
Method: other (calculated)
Remark: The reported value is 3×10^{-13} Pa.

Cites estimates calculated by Lyman (see References).
Source: HERA 2002; Lyman 1985.
Test substance: C12 LAS (CAS #25155-30-0)
Reliability: (4) not assignable

21-FEB-2003 (18) (43)

2.5 Partition Coefficient

log Pow: = 2 at 23 degree C
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year: 1981
GLP: no
Remark: IUCLID cites source as Shell Chemical U.K. Ltd. Chester. No report available for review.
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Reliability: (2) valid with restrictions

05-DEC-2001 (27)

log Pow: = 1.96
Method: other (calculated): Leo and Hansch
Year: 1971
GLP: no data
Remark: Original data from Leo, A., Hansch, C., and Elkins, D. 1971. Chem. Rev. 71:525-616.
Source: Hand and Williams 1987.
Test substance: Sodium dodecylbenzenesulfonate as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
Based on data from standard reference source.
11-OCT-2001 (16)

log Pow: = 2.52
Method: other (calculated): Leo and Hansch
Year: 1971
GLP: no data
Remark: Original data from Leo, A., Hansch, C., and Elkins, D. 1971. Chem. Rev. 71:525-616.
Source: Hand and Williams 1987.
Test substance: Sodium tridecylbenzene sulfonate as surrogate for benzene sulfonic acid, tridecyl- (25496-01-9)
Reliability: (2) valid with restrictions
Based on data from standard reference source.
11-OCT-2001 (16)

log Pow: = 3.32
Method: other (calculated)
Year:
GLP: no
Remark: Calculated using the method of Leo and Hansch (1979) modified to take into account the various phenyl positions along the linear alkyl chain as per Roberts (1991).
Source: HERA 2002; Roberts 1991; Leo and Hansch 1979.
Test substance: C11.6 LAS
Reliability: (4) not assignable
21-FEB-2003 (18) (39) (65)

2.6.1 Water Solubility

Value: 400000 mg/l at 20 degree C
GLP: no
Remark: The IUCLID Data Sheet cites a Shell Chemical report indicating that the substance is miscible in water up to 40%.
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Reliability: (2) valid with restrictions
05-DEC-2001 (27)

Value: = 300000 mg/l at 20 degree C
pH: > 9
GLP: no data
Remark: The IUCLID Data Sheet cites a Shell Chemical report indicating that the substance is miscible in water up to 40%.
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
04-DEC-2001 (28)

Result: The reported pKa for all of the LAB sulfonic acids is < 1.
Source: Noeller 1966; Lide 1990.
Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5), Benzene sulfonic acid, dodecyl- (27176-87-0), and Benzene sulfonic acid, tridecyl- (25496-01-9)
Reliability: (2) valid with restrictions
11-OCT-2001 (40) (50)

Value: > 250 g/l
Qualitative: miscible
GLP: no data
Remark: The study shows that 25% solutions (250 g/L) of various LASs have cloud clear points (i.e., form clear solutions) at temperatures of 2-21°C or above. Therefore, the results demonstrate that 25% solutions of LAS are soluble at room temperature.
Source: Cohen 1995.
Test substance: Various LASs made from four commercial LABs, average alkyl chain length = 11.6
Reliability: (2) valid with restrictions
21-FEB-2003 (3)

pH: = 10
GLP: no data
Remark: Reported pH value is 10.0 +/- 1.0 (1% solution).
Source: Huntsman 2002.
Test substance: C10-14 monoalkylbenzene sulfonic acid, sodium salt (CAS #85117-50-6); mean molecular weight = 348, average alkyl chain length = C12.0
Reliability: (4) not assignable
21-FEB-2003 (22)

2.6.2 Surface Tension

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.7 Flash Point

Value:

Type:

Method:

Year:

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.8 Auto Flammability

Value:

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.9 Flammability

Result:

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.10 Explosive Properties

Result:

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.11 Oxidizing Properties

Result:

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.12 Additional Remarks

Memo: None
11-OCT-2001

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .00000000001352 cm3/(molecule * sec)
Degradation: = 50 % after 8.6 hour(s)
Method: other (calculated): EPISuite, Version 3.10
Year: **GLP:**
Test substance:
Source: USEPA 2000.
Test substance: Benzene sulfonic acid, undecyl (50854-94-9) as a surrogate for Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5). The C11 sulfonic acid was used because it more closely approximates the average alkyl chain length for the C10-16 material, which ranges from 11.0 to 11.8. The EpiSuite model calculates the C10-16 material based on its lowest alkyl chain length, which is C10. This half-life value was 9.5 hours.
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
21-JAN-2002 (76)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .00000000001636 cm3/(molecule * sec)
Degradation: = 50 % after 7.9 hour(s)
Method: other (calculated): EPISuite, Version 3.10
Year: **GLP:**
Test substance: other TS: Benzene sulfonic acid, dodecyl (27176-87-0). The EPISuite model calculates this material based on a C12 alkyl chain length rather than the full range of carbon chain lengths present.
Source: USEPA 2000.
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
21-JAN-2002 (76)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .00000000001777 cm3/(molecule * sec)
Degradation: = 50 % after 7.2 hour(s)
Method: other (calculated): EPISuite, Version 3.10
Year: **GLP:**
Test substance: other TS: Benzene sulfonic acid, tridecyl (25496-01-9). The EPISuite model calculates this material based on a C13 alkyl chain length rather than the full range of carbon chain lengths present.
Source: USEPA 2000.
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
21-JAN-2002 (76)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .00000000001339 cm3/(molecule * sec)
Degradation: = 50 % after 7.9 hour(s)
Method: other (calculated): EPISuite, Version 3.10
Year: **GLP:**
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (25155-30-0 et al.). The modeled material was a C12-LAS.
Source: USEPA 2000.
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
21-JAN-2002 (76)

Type: water
Light source: other: Mercury vapor lamp
Light spect.: = 200 - 350 nm
DIRECT PHOTOLYSIS
Degradation: > 95 % after 20 minute(s)
Method:
Year: **GLP:** no data
Test substance: other TS: LAS; activity: 95% (CAS #25155-30-0)
Method: A series of photodegradation studies were conducted. Aqueous solution of LAS (pH 6.75) were passed through an irradiated tubular flow reactor. Reaction rates were obtained for both non-sensitized conditions and when ferric perchlorate (0.04 to 3.15 x 10⁻⁴ g-mole/L) was used as a sensitizer. A Hanovia 1200-watt mercury-vapor lamp was the source of radiation. The LAS concentration was determined by the methylene blue method.
Remark: Rapid photodegradation occurred in indirect photolysis degradation. Complete conversion of LAS to intermediates at an average residence time as low as 1 minute. The maximum conversion to CO₂ was obtained at a residence time of 20 minutes and corresponded to 7 moles CO₂ per mole of LAS. Reaction rate increases by two orders of magnitude in presence of ferric perchlorate. Half order kinetics with respect to

light intensity and LAS concentration explained the data for nonsensitized conditions. An appropriate rate equation could be derived by assuming a second-order deactivation of light-activated LAS molecules. The sensitized reaction was believed to occur by abstraction of hydrogen atoms from LAS by hydroxyl radicals. Hydroxyl radicals presumably are produced by an electron-transfer reaction involving light-activated ferric ions. The mechanism is complex; over-all kinetics indicated a first-order effect of (Fe+3), 1.2 order in light intensity, and maxima in the rate for intermediate LAS and O₂ concentrations.

Initial LAS concentration was 60 to 182 mg/L.

Source: Matsuura and Smith 1970.
Reliability: (2) valid with restrictions
20-FEB-2003

(45)

3.1.2 Stability in Water

Type: abiotic
Method:
Year: **GLP:** no data
Test substance: other TS: C10-13 alkylbenzene sulfonic acid, sodium salt (CAS #68411-30-3)
Remark: LAS is stable in water. LAS can be decomposed at extreme conditions such as elevated temperatures in the presence of inorganic acids such as phosphoric, sulphuric and hydrochloric acid, e.g.: 60-70% sulphuric acid at 140 - 190 degree C or with concentrated HCl in a sealed container at 150 - 200 degree C. Information as cited in IUCLID Data Sheet for CAS #68411-30-3.
Source: Cross and Dekker 1977.
Reliability: (4) not assignable
21-FEB-2003

(5)

3.1.3 Stability in Soil

Type: **Radiolabel:**
Concentration:
Cation exch.
capac.
Microbial
biomass:
Method:
Year: **GLP:**
Test substance:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

3.2 Monitoring Data (Environment)

Type of
measurement:
Medium:
Remark: None
02-NOV-2001

3.3.1 Transport between Environmental Compartments

Type:
Media:
Method:
Year:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

3.3.2 Distribution

Media:
Method: other (calculation): Fugacity Level III
Year:
Remark: Mass Distribution by Environmental Compartment

Air: 1.13%
Water: 31.7%
Soil: 63.3%
Sediment: 3.81%

Source: USEPA 2000.
Test substance: Benzene sulfonic acid, undecyl (50854-94-9), which best represents the actual alkyl chain length (11.0-11.8) of Benzene sulfonic acid, C10-16 alkyl derivatives (68584-22-5)
Reliability: (2) valid with restrictions
21-JAN-2002 (76)

Media:
Method: other (calculation): Fugacity Level III
Year:
Remark: Mass Distribution by Environmental Compartment

Air: 1.03%
Water: 29.1%
Soil: 59.7%
Sediment: 10.0%

Source: USEPA 2000.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
02-NOV-2001 (76)

Media:
Method: other (calculation): Fugacity Level III
Year:
Remark: Mass Distribution by Environmental Compartment

Air: 0.878%
Water: 23.3%
Soil: 52.4%
Sediment: 23.4%

Source: USEPA 2000.
Test substance: Benzene sulfonic acid, tridecyl- (25496-01-9)
Reliability: (2) valid with restrictions
02-NOV-2001 (76)

Media:
Method: other (calculation): Fugacity Level III
Year:
Remark: Mass Distribution by Environmental Compartment

Air: 1.14%
Water: 34.1%
Soil: 64.4%
Sediment: 0.367%

Source: USEPA 2000.
Test substance: Linear Alkylbenzene Sulfonate (LAS) (25155-30-0 et al.) (The modeled material was a C12-LAS)
Reliability: (2) valid with restrictions
20-FEB-2003 (76)

3.4 Mode of Degradation in Actual Use

Memo: The LAB sulfonic acids are intermediates in the production of LAS.
11-OCT-2001

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge
Concentration: 11.3 mg/l related to DOC (Dissolved Organic Carbon)
Contact time: 28 day
Degradation: = 94 % after 28 day
Result: readily biodegradable
Method: other: OECD DOC-Die away test (EG - Richtlinie 92/69 EWG, Tiel II, C.4-A)
Year: 1992 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Source: Kurtin 1994.
Reliability: (1) valid without restriction
05-DEC-2001 (33)

Type: aerobic
Inoculum: domestic sewage
Concentration: 11.6 mg/l related to Test substance
Contact time: 37 day
Degradation: = 92 % after 37 day
Method: other: Modified coupled units test
Year: 1991 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Source: Kurtin 1994; Schoberl 1991.
Reliability: (1) valid without restriction
04-DEC-2001 (34) (67)

Type: aerobic
Inoculum: activated sludge
Concentration: 10 mg/l related to DOC (Dissolved Organic Carbon)
20 mg/l related to DOC (Dissolved Organic Carbon)
Contact time: 28 day
Degradation: = 69 % after 28 day
Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 1992 **GLP:** no data
Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)
Remark: % degradation refers to mineralization.
Source: Stepan; OECD 1992.
Reliability: (2) valid with restrictions
03-JUL-2001 (61) (69)

Type: aerobic
Inoculum: activated sludge, domestic, non-adapted
Concentration: 10.8 mg/l related to DOC (Dissolved Organic Carbon)
Contact time: 28 day
Degradation: = 93 % after 28 day
Result: readily biodegradable
Kinetic: 7 day = 59 %
14 day = 73 %
21 day = 82 %
Method: other: Directive 79/831/EEC, Appendix V, C.4-A. DOC Die-Away Test
Year: 1990 **GLP:** yes
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et al.)
Remark: The many biodegradation studies for LAS all report that LAS is readily biodegradable.
Source: Huels 1993.
Reliability: (2) valid with restrictions
11-OCT-2001 (21)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: Not an HPV Challenge endpoint.
21-MAR-2003

3.7 Bioaccumulation

Species: Leuciscus idus melanotus (Fish, fresh water)
Exposure period: 3 day
Concentration:
BCF: = 130
Elimination:
Method: other: Golden ide were exposed to a constant water concentration of the dissolved test material for 3 days.
Year: **GLP:** no
Test substance: other TS: Dodecylbenzenesulphate sodium salt as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Remark: A BCF of 130 indicates a moderate affinity for uptake in fish tissues. However, uptake into tissues may be offset by metabolism and/or excretion.
Source: Freitag et al. 1985.
Reliability: (1) valid without restriction
11-OCT-2001 (14)

Species: Pimephales promelas (Fish, fresh water)
Exposure period: 48 hour(s)
Concentration: 2.7
BCF: = 22 - 87
Elimination: yes
Method: OECD Guide-line 305 E "Bioaccumulation: Flow-through Fish Test"
Year: 1981 **GLP:** yes
Test substance: other TS: LAS (C10-13), tested individually and as mixtures, activity: >97.4%
Method: The exposure phase in Experiment A was 48-hours. The exposure phase in Experiments B-D ranged from 168 to 192 hours. Fish were then transferred to untreated water for the depuration phase.
Remark: BCF values ranged between 2-1000 L/kg with BCFs increasing with increasing alkyl chain length. To address differences in composition of mixtures, bioconcentration potential was evaluated for a mixture typical of LAS in European detergent formulations (C10 12%, C11 29%, C12 34%, C13 24%; average alkyl chain length = C11.6) and a mixture typical of LAS in filtered Mississippi river water (C10 45%, C11 23%, C12 23%, C13 2%; average chain length = C10.8). The respective BCFs were 87 and 22 L/kg at concentrations of 2.7 and 4.1 uM, indicating that environmental processes decrease the bioconcentration potential of LAS.
Source: Tolls 1997; OECD 1981.
Test condition: The type of test was measured and flow-through.
Reliability: (2) valid with restrictions
20-FEB-2003 (51) (74)

3.8 Additional Remarks

Memo: None
02-NOV-2001

AQUATIC ORGANISMS**4.1 Acute/Prolonged Toxicity to Fish**

Type: flow through
Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:**
LC50: = 5.6
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: The LC0 and LC100 were 4 and 8 mg/L, respectively.
Source: Kurtin 1997; OECD 1984.
Reliability: (1) valid without restriction
02-JUL-2001 (36) (58)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: = 4
LC50: = 4.1
LC100: = 4.3
Method: other: DIN 38412 Part 15
Year: **GLP:** yes
Test substance: other TS: n-dodecylbenzenesulfonate as a surrogate for benzene sulfonic acid dodecyl- (27176-87-0)
Source: Knie et al. 1983
Reliability: (1) valid without restriction
03-JUL-2001 (7) (30)

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: = 10
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1992 **GLP:** yes
Test substance: other TS: Dodecylbenzenesulfonate-sodium salt as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Source: OECD 1992; IUCLID 1995.
Reliability: (2) valid with restrictions
Company GLP report cited in IUCLID Data Sheet but not available for review.
03-JUL-2001 (19) (60)

Type: other: daily renewal
Species: *Salmo gairdneri* (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: = 4.3
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1992 **GLP:** no
Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)
Remark: LC50 is geometric mean of lower (3.2 mg/L) and upper (5.6 mg/L) limits from a series of studies investigating the reduction in number of individuals needed for testing.
Source: OECD 1992; Douglas et al. 1986.
Reliability: (1) valid without restriction
03-JUL-2001 (10) (60)

Type: static
Species: *Salmo gairdneri* (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: = 3
Method:
Year: 1981 **GLP:** yes
Test substance: other TS: Dobanic acid 102 (linear alkyl benzenesulfonic acid, C10-13) as a surrogate for Benzene sulfonic acid, tridecyl- (25496-01-9)
Method: Five aquaria were filled with a series of concentrations between 0.2 and 5 mg/l of Dobanic acid 102. One aquarium was a control. Five fish were placed in each aquarium. The concentration, temperature, and pH were kept constant.
Source: Stephenson 1981.
Reliability: (1) valid without restriction
03-JUL-2001 (70)

Type: semistatic
Species: *Salmo gairdneri* (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: = 5.8
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1992 **GLP:** no data
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et al.)
Remark: Analysis showed 92% of nominal concentration, tap water, water hardness; 96-120 mg/L CaCO₃, pH 6.8-7.3, daily renewal, 14.5-16 C; life-stage: 5 months.
Source: Procter & Gamble 1991; OECD 1992.
Reliability: (1) valid without restriction
11-OCT-2001 (60) (63)

Type:
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period:
Unit: mg/l **Analytical monitoring:**
LC50: = 3
Method:
Year: **GLP:**
Test substance: other TS: LAS normalized to C11.6
Remark: Mean LC50 for bluegill sunfish was derived from a total of 88 records compiled from several literature reviews.
Source: van de Plassche et al. 1999.
Reliability: (4) not assignable
21-FEB-2003 (77)

Type:
Species: Pimephales promelas (Fish, fresh water)
Exposure period:
Unit: mg/l **Analytical monitoring:**
LC50: = 3.2
Method:
Year: **GLP:**
Test substance: other TS: LAS normalized to C11.6
Remark: Mean LC50 for fathead minnow was derived from a total of 35 records compiled from several literature reviews.
Source: van de Plassche et al. 1999.
Reliability: (4) not assignable
21-FEB-2003 (77)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: = 5.2
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: other TS: 4-C10-13 Alkylbenzene sulfonic acid (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Source: Kurtin 1995; OECD 1984.
Reliability: (1) valid without restriction
21-FEB-2003 (35) (62)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: = 9.3 - 11.6
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: other TS: See Remark
Remark: The toxicity values of the LAB sulfonic acids are in the same order as their sodium salts. As the chain length gets longer, the LC50 decreases. Three LAB sulfonic acids of varying chain lengths neutralized with caustic soda to obtain the sodium salt derivative were tested. Acid A had 48.4% of its weight in the C11 range and the majority its chain length ranged from C10-C13. Acid B had 49.4% of its weight in the C11 range and 31.7% of its weight in the C12 range. The majority of its chain length ranged from C10 to C12. Acid C had the majority of its chain length in the C10 to C13 range, almost evenly distributed between C11 and C12.
Result: Acid A had a LC50 of 11.6 mg/L, acid B 10.8 mg/L, and acid C 9.3 mg/L.
Source: Verge 2000; OECD 1984.
Reliability: (1) valid without restriction
21-FEB-2003 (57) (79)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = 2.9
Method: other: The test solution was added to dishes in concentrations ranging from 0.3-20 mg/l with controls. Ten organisms were added to each dish. Immobilised organisms were recorded at 24 and 48 hours.
Year: 1981 **GLP:** yes
Test substance: other TS: Dobanic acid (linear alkyl benzenesulfonic acid, C10-13) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Source: Stephenson 1981.
Reliability: (1) valid without restriction
21-FEB-2003 (70)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC0: = 6
EC50: = 12
EC100: = 14
Method: other: DIN 38412 Part 11
Year: **GLP:** yes
Test substance: other TS: n-dodecylbenzenesulfonate as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Source: Knie et al. 1983.
Reliability: (1) valid without restriction
20-FEB-2003 (6) (30)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: = 5.88
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: **GLP:** no data
Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)
Source: Galassi et al. 1992; EEC Directive.
Reliability: (2) valid with restrictions
Data as cited in IUCLID data sheet.
20-FEB-2003 (9) (15)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: = 4.3
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance:
Source: Verge et al. 2000; OECD 1984.
Test substance: The substance tested was derived from a LAB product with 67.0% of its weight in the C13 range. The rest of the weight is spread over the C10-C14 range. Used as a surrogate for benzene sulfonic acid, tridecyl- (25496-01-9).
Reliability: (1) valid without restriction
21-FEB-2003 (57) (79)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = 6.8
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: 1984 **GLP:** yes
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et al.)
Source: EEC Directive 1984.
Reliability: (1) valid without restriction
21-FEB-2003 (9)

Species: Daphnia magna (Crustacea)
Exposure period:
Unit: mg/l **Analytical monitoring:**
EC50: = 4.1
Method:
Year: **GLP:**
Test substance: other TS: C10-13 LAS (CAS #68411-30-3)
Remark: D. magna was selected as the representative test organism of the toxicity of LAS to invertebrates. The value is a mean of 17 records of commercially representative LAS with C10-13 alkyl chain lengths and average carbon numbers of C11.6 and C11.8.
Source: HERA 2002.
Reliability: (4) not assignable
21-FEB-2003 (18)

Species: Daphnia magna (Crustacea)
Exposure period:
Unit: mg/l **Analytical monitoring:**
EC50: = 4.7
Method:
Year: **GLP:**
Test substance: other TS: LAS normalized to C11.6
Remark: EC50 is geometric mean of 139 records compiled from literature reviews. Values range from 0.26 to 55 mg/L. This large range is caused by differences in the LAS tested with respect to alkyl chain and/or phenyl isomer distribution and differences in test design.
Source: van de Plassche et al. 1999.
Reliability: (4) not assignable
21-FEB-2003 (77)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: = 36
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: The reported EC50 is for growth rate. The 72-hr EC50 for biomass was also tested in this experiment and determined to be 14 mg/L for this substance.
Source: Kurtin 1994; OECD 1984.
Reliability: (1) valid without restriction
21-FEB-2003 (32) (56)

Species: Selenastrum capricornutum (Algae)
Endpoint: growth rate
Exposure period: 4 day
Unit: mg/l **Analytical monitoring:** no
EC50: = 170
Method: other: Twelve flasks were filled with quantities of test solution ranging from 2-200 mg/l. Six flasks served as controls. Algae was added to each container. Cell counts were made after 2 and 4 days.
Year: 1981 **GLP:** yes
Test substance: other TS: Dobanic acid (linear alkyl benzenesulfonic acid, C10-13) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Source: Stephenson 1981.
Reliability: (1) valid without restriction
21-FEB-2003 (70)

Species: Haematococcus pluvialis (Algae)
Endpoint: other: inhibition of oxygen production
Exposure period: 4 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = 50
Method: other: Based on the procedure by Tumpling. The initial cell density was 80,000 cells/mL.
Year: **GLP:** yes
Test substance: other TS: n-dodecylbenzenesulfonate as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Source: Knie et al. 1983.
Reliability: (1) valid without restriction
20-FEB-2003 (30)

Species: Selenastrum capricornutum (Algae)
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: = 29
Method: other: EPA method
Year: 1985 **GLP:** no
Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)
Source: Galassi et al. 1992; EPA 1985.
Reliability: (2) valid with restrictions
Data as cited in IUCLID data sheet.
20-FEB-2003 (15) (75)

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** no
NOEC: = 30
EC50: = 163
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 **GLP:** no data
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et al.)
Source: Verge 1996; OECD 1984.
Reliability: (2) valid with restrictions
21-FEB-2003 (56) (78)

Species:
Endpoint:
Exposure period:
Unit: mg/l **Analytical monitoring:**
IC50 : = 9.1
Method:
Year: **GLP:**
Test substance: other TS: C10-13 LAS (CAS #68411-30-30)
Remark: Data are for various algae species. The value is a geometric mean of 12 records of commercially representative LAS with C10-13 alkyl chain lengths and average carbon number of C11.6 and C11.8.
Source: HERA 2002.
Reliability: (4) not assignable
21-FEB-2003 (18)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type:
Species:
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: Not an HPV Challenge endpoint.
21-MAR-2003

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: other: Brachydanio rerio, Pimephales promelas, Poecilia reticulata, Oncorhynchus mykiss, and Tilapia mossambica
Endpoint: other: growth
Exposure period: 28 day
Unit: mg/l **Analytical monitoring:** no
NOEC: = .25 - 3.2
Method:
Year: **GLP:** no data
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et al.)
Remark: All data were from tests conducted on commercial LAS with C10-13 alkyl chains and average carbon lengths of C11.6 and C11.8. The NOEC values have been normalized using QSARs to the average structure of C11.6 LAS.
Result: The article compiles the no observed effect concentration (NOEC) values for many tests conducted on an assortment of species. The following table shows the geometric mean NOEC values for each fish species (n = number of studies included for each species).

Species	Geometric mean NOEC (mg/L)	n
Brachydanio rerio	2.3	1
Pimephales promelas	0.87	14
Poecilia reticulata	3.2	1
Oncorhynchus mykiss	0.34	7
Tilapia mossambica	0.25	1

Source: van de Plassche et al. 1999.
Reliability: (4) not assignable
21-MAR-2003 (77)
03

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Endpoint:
Exposure period:
Unit: mg/l **Analytical monitoring:**
NOEC: = 1.4
Method:
Year: **GLP:**
Test substance: other TS: LAS normalized to C11.6
Remark: NOEC is geometric mean of 12 records compiled from literature reviews and normalized to C11.6.
Source: van de Plassche et al. 1999.
Reliability: (4) not assignable
21-FEB-2003 (77)

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type:
Species:
Endpoint:
Exposure period:
Unit:
Method:
Year: GLP:
Test substance:
Remark: Not an HPV Challenge endpoint.
20-FEB-20
03

4.6.2 Toxicity to Terrestrial Plants

Species:
Endpoint:
Expos. period:
Unit:
Method:
Year: GLP:
Test substance:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

Species:
Endpoint:
Expos. period:
Unit:
Method:
Year: GLP:
Test substance:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

4.7 Biological Effects Monitoring

Memo: Not an HPV Challenge endpoint.
20-FEB-2003

4. Ecotoxicity

date: 27-MAR-2003
Substance ID: LABSA

4.8 Biotransformation and Kinetics

Type:

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

4.9 Additional Remarks

Memo:

None
11-OCT-2001

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: other: rat, Wistar
Sex: male/female
Number of Animals: 10
Vehicle: other: none
Value: = 1470 mg/kg bw
Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1981 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: Five of each sex per dose level were tested. Test duration was 14 days. The dose range was 1250-1990 mg/kg.
Source: Murmann 1984; OECD 1981.
Reliability: (1) valid without restriction
21-FEB-2003 (46) (52)

Type: LD50
Species: other: rat, Sprague-Dawley CD
Sex: male/female
Number of Animals: 9
Vehicle: other: distilled water
Value: = 775 mg/kg bw
Method: other: Safepharm Standard Test Method Number 513.01
Year: 1998 **GLP:** yes
Test substance: other TS: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Method: A group of three fasted males was treated with the starting dose (2000 mg/kg bw). As the females dosed with 2000 mg/kg bw died, a further three fasted males and three fasted females were treated with the dose level 300 mg/kg bw. The test material was administered orally as a solution in distilled water. The animals were observed 1/2, 1, 2, and 4 hours after dosing and then once daily for up to 14 days. Bodyweights were recorded on Day 0 (day of dosing) and on Days 7 and 14 or at death. At the end of the observation period the surviving animals were killed by cervical dislocation and all animals were subject to gross necropsy.
Remark: LD50 value is geometric mean between 300 and 2000 mg/kg. Three females were found dead one day after dosing at the 2000 mg/kg bw dose level. There were no deaths at the 300 mg/kg bw dose level. No clinical signs of toxicity were noted in animals treated with 300 mg/kg bw. The surviving animals showed expected gains in body weight over the study period. Abnormalities noted at necropsy of animals that died during the study were abnormally red lungs, dark liver, and dark kidneys.
Source: Hempstock 1998.

Reliability: (1) valid without restriction
21-FEB-2003 (17)

Type: LD50
Species: other: rat, Wistar
Sex: male/female
Number of Animals:
Vehicle: no data
Value: = 500 - 2000 mg/kg bw
Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1987 **GLP:** yes
Test substance: other TS: Dodecylbenzenesulfonate, sodium salt as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Source: OECD 1987; IUCLID 1995.
Reliability: (2) valid with restrictions
Company reported GLP study listed in IUCLID Data Set but not available for review.

02-JUL-2001 (20) (59)

Type: LD50
Species: rat
Sex: male/female
Number of Animals: 10
Vehicle:
Value: = 1080 mg/kg bw
Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1981 **GLP:** no
Test substance: other TS: Marlon A 386 (CAS #68411-30-3) C10-13 LAS, average alkyl chain length = C11.6; Activity: 86%
Method: Five male and five female rats were given LAS doses of 1075, 1220, 1360, 1710 or a control by gavage. Body weight and other signs were measured on days 7 and 14. Temperature was maintained at 20+/-1°C with a 12 hr light-dark cycle. Animals were observed for 14 days after dosing.
Remark: Symptoms beginning about 30 minutes past application included diarrhea, squatting attitude, breathing difficulties, nose bleeding, ataxia, and lethargy. These symptoms had disappeared in surviving animals by 120 hours. Virtually all animals died in doses of 1220 mg/kg and above. Note that all doses are corrected for 86% activity. The original doses were 1250, 1415, 1580 and 1990 mg/kg.
Source: Murmann 1984a.
Reliability: (2) valid with restrictions
21-FEB-2003 (49)

Type: LD50
Species: other: Rat, CFY (Sprague-Dawley origin)
Sex: male/female
Number of Animals: 10
Vehicle:
Value: = 1980 mg/kg bw
Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: **GLP:** yes
Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na).
Method: Five male and five female rats were given single doses by gavage at 1500, 2350 and 3760 mg/kg bw. Rats were housed in cages grouped by sex and given standard laboratory diet and water ad libitum. Mean daily temperature was maintained at 21-22°C at a mean relative humidity of 56%. Lighting was on a 12 hrs dark and 12 hrs light photoperiod. Animals were observed for 14 days after dosing.
Remark: Four rats from each of the two lowest concentrations and all rats from the highest concentration died. All deaths occurred between 6 and 23 hours after dosing. Signs of reaction to treatment included pilo-erection, hunched posture, abnormal gait (waddling), lethargy, decreased respiratory rate, ptosis, pallor of the extremities, and diarrhea. All surviving animals appeared to recover completely by day 4. Autopsy of rats that died revealed isolated cases of pallor of the kidneys or spleen. Terminal necropsy findings for survivors were normal. Note that all doses are corrected for 47% activity. The original doses were 3200, 5000, and 8000 mg/kg.
Source: Kynoch 1986a.
Test substance: Activity 47%. Average alkyl chain length = C11.2 Clear yellow liquid.
Reliability: (1) valid without restriction
21-FEB-2003 (37)

5.1.2 Acute Inhalation Toxicity

Type: other: Approximate Lethal Concentration (ALC)
Species: other: Rat Crl: CD (SD) BR
Sex: male
Number of Animals: 6
Vehicle:
Exposure time: 4 hour(s)
Value:
Method: other
Year: 1992 **GLP:** no data
Test substance: other TS: LAS (CAS #25155-30-0); activity 98%
Method: Groups of six male 8-week old rats were restrained in perforated, stainless steel cylinders with conical nose pieces. Exposure was nose-only to an aerosol atmosphere for 4 hours. After exposure, rats were returned to their cages and observed for clinical signs for 14 days. Mean measured

Remark:

concentrations in the test chambers were 65, 120, 260, and 310 mg/m³. Chamber temperature ranged between 25-26°C.

The ALC is defined as the lowest atmospheric concentration generated that caused death in 1 or more rats either on the day of exposure or within 14 days post exposure. No mortality occurred at concentrations up to 260 mg/m³. At 310 mg/m³, one rat died during exposure and 2 rats died one day post exposure. The test material is considered moderately toxic by inhalation. However, it is important to note that this laboratory exposure is not representative of the possible LAS exposure during actual use. In this study, animals were given high exposures to respirable-sized particles. Spray products containing LAS are designed to produce large particle sizes. These large particles are needed for efficient delivery of the spray to the surface being cleaned. This results in particle sizes that are much larger than the respirable particle sizes used in testing and therefore would not be able to reach far into the lungs where effects could occur. Given this lack of relevance to real-world exposure potential, the use of this study for risk assessment purposes is limited.

Result:

310 mg/m³ of particulate

Source:

Kinney 1985.

Reliability:

(2) valid with restrictions

21-FEB-2003

(29)

5.1.3 Acute Dermal Toxicity

Type:

LD50

Species:

rabbit

Sex:**Number of****Animals:**

6

Vehicle:**Value:**

= 2000 mg/kg bw

Method:

other: Test material was applied to shaved area of back of 6 rabbits at two doses: 2000 mg/kg (undiluted) and 212 mg/kg (2% aqueous dilution). The areas were covered with plastic and left in contact with test material for 24 hours.

Year:

GLP: no

Test substance:

other TS: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)

Remark:

All of the animals exposed to the 212 mg/kg survived. Mortality occurred in three out of six rabbits exposed to the undiluted dose. No untoward behavioral reactions were observed. Necropsy did not reveal any gross pathological alterations. Local skin reactions included erythema, mild edema and mild desquamation at 212 mg/kg and chemical burns, severe edema and necrosis at 2000 mg/kg.

Result:

LD50 = 2000 mg/kg bw (undiluted); LD50 > 212 mg/kg bw (2% aqueous dilution)

Source:

Kretchmar 1972.

Reliability:

(1) valid without restriction

21-FEB-2003

(31)

Type: LD50
Species: other: Rat, CFY (Sprague-Dawley origin)
Sex: male/female
Number of Animals: 10
Vehicle:
Value: > 2000 mg/kg bw
Method: OECD Guide-line 402 "Acute dermal Toxicity"
Year: **GLP:** yes
Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na). activity 47%. Average alkyl chain length = C11.2. Yellow, viscous liquid.
Method: Five male and five female rats were exposed to 2000 mg/kg in a limit test. The test substance was applied to clipped intact skin in the dorso-lumbar region and covered with gauze held in place with an impermeable dressing. The dressing was removed after 24 hours and the treated area of the skin washed with warm water and blotted dry. Observations for dermal irritation were made daily for 14 days.
Remark: There were no deaths or signs of a systemic reaction following a single dermal application at 2000 mg/kg bw. Well defined or slight erythema and slight oedema were observed at all test sites after removal of the occlusive dressing on Day 2. All test sites were entirely covered by scab formation from Day 7. Sloughing from the scabbed skin began at various times between Day 7 and Day 12 and was completed before termination. Low bodyweight gains or loss of body weight were recorded for one male and three females in Day 8. Two of the same females and a third female also showed low bodyweight gain between Days 8 and 15.
Source: Kynoch 1986b.
Reliability: (1) valid without restriction
21-FEB-2003 (38)

5.1.4 Acute Toxicity, other Routes

Type:
Species:
Sex:
Number of Animals:
Vehicle:
Route of admin.:
Value:
Method: **GLP:**
Year:
Test substance:
Remark: Not a required OECD or HPV endpoint.
08-FEB-2001

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration: .5 other: mL

Exposure:
Exposure Time: 4 hour(s)
Number of Animals: 6
PDII:
Result: highly irritating
EC classificat.: irritating
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1981 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: The shaved treated area was covered for the first 4 hours. Observations were made after 1, 24, 48, 72 hours and 6, 9, and 14 days. The irritation index was 5.25.
Source: Murman 1984; OECD 1981.
Reliability: (1) valid without restriction
20-FEB-2003 (48) (53)

Species: rabbit
Concentration: .5 other: mL

Exposure:
Exposure Time: 4 hour(s)
Number of Animals: 6
PDII:
Result: corrosive
EC classificat.: irritating
Method: Draize Test
Year: 1965 **GLP:**
Test substance: other TS: Benzene sulfonic acid dodecyl- (27176-87-0)
Method: The test material was applied as submitted to the intact skin and covered with a "1 x 1" gauze patch held in place with saran wrap. At the end of 4 hours, the coverings were removed and the area examined for skin irritation and corrosion. Examinations were repeated at 24 and 48 hours and scored according to Draize 1965.
Remark: The primary dermal irritation scores were 3.4, 6.3, and 7.0 at 4, 24, and 48 hours, respectively.
Source: Thompson 1980.
Reliability: (1) valid without restriction
02-NOV-2001 (1) (11) (71)

Species: other: New Zealand albino rabbits
Concentration: .5 other: mL

Exposure:
Exposure Time: 4 hour(s)
Number of Animals: 6
PDII:
Result: moderately irritating
EC classificat.:
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: GLP: yes
Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na). Activity 47%. Average alkyl chain length = C11.2. Clear yellow liquid.

Method: A 0.5 ml aliquot of P-500 N-Na was applied under a 2.5 cm2 gauze pad to an approximate 10 cm2 area of clipped intact skin of 3 rabbits. Each treatment site was occluded with an elastic adhesive dressing for four hours, after which the dressing was removed and the area washed with distilled water. Examination of the treated skin was made approximately 30 minutes after removal of the patch and daily through 14 days. Grading and scoring of the dermal reactions was performed using the standard numerical scoring system.

Remark: Well defined to moderate skin reactions were observed in all three animals following removal of the bandages. Desquamation of the stratum corneum was observed in all three animals. The reaction in all three animals gradually ameliorated from Days 5, 10 and 11, respectively, and had all resolved completely in one animal by Day 12.

Source: Liggett and Parcell 1986a.
Reliability: (1) valid without restriction
21-FEB-2003 (41)

5.2.2 Eye Irritation

Species: rabbit
Concentration: .1 other: mL
Dose:
Exposure Time: 144 hour(s)
Comment:
Number of Animals: 6
Result: moderately irritating
EC classificat.: irritating
Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1981 GLP: no
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)

Remark: Treatment was to the right eye with lower lid removed. The left eye was untreated. The eyes were not washed out during the test. Observations were made at 1, 24, 48, and 72 hours

and at 6 days after application. The total irritation index was 46.9.

Source: Murmann 1984; OECD 1981.

Reliability: (1) valid without restriction (47) (54)

20-FEB-2003

Species: other: New Zealand albino rabbits

Concentration: .1 other: mL

Dose:

Exposure Time:

Comment:

Number of Animals: 9

Result: irritating

EC classificat.:

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"

Year: 1981 **GLP:** yes

Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na). Activity 47%. Average alkyl chain length = C11.2. Clear yellow liquid.

Method: Nine rabbits received a 0.1 mL aliquot of P-500 N-Na placed into the lower everted lid of one eye per animal. For three rabbits the eyelids were then gently held together for one second before releasing. For three other rabbits the eyes were irrigated with water for 5 minutes following a 4-second exposure. For the remaining three rabbits the eyes were irrigated for 5 minutes following a 30-second exposure. Eyes were examined after 1 hour and 1, 2, 3, 4, 7, 14 and 21 days after exposure. Grading was performed using the standard scoring system.

Remark: The following results were noted:

1) Three animals without any rinsing: averaged irritation scores (24, 48, 72 hours) for each animal: cornea 2.3, 1.7, 2; iris: 1.3, 0, 0; conjunctivae redness: 3, 1.7, 2; conjunctivae chemosis: 3, 2, 2. In the first animal the effects were persistent at day 14.

2) Three animals with rinsing for five minutes following a 30 second exposure: averaged scores: cornea 0.7, 1, 1.3; iris: 0, 0.7, 0.3; conjunctivae redness: 1.7, 2, 1.3; conjunctivae chemosis: 2, 1.3, 2. The eyes were normal 7 or 14 days after instillation.

3) Three animals with rinsing for five minutes following a 4 second exposure: averaged scores: cornea 0.7, 2.3, 0.7; iris: 0, 0, 0; conjunctivae redness: 1.7, 1.7, 1; conjunctivae chemosis: 1.3, 2, 1. The eyes were normal 7 days after instillation.

Findings lead to a definition of irritating for LAS at 47% applied without rinsing, irritating (even if with lower effects, mainly as cornea opacity and conjunctivae redness) with rinsing after 30 second of exposure, and not irritating

with rinsing after 4 second of exposure.
Overall, instillation of P-500 N-Na into the eyes of rabbits elicited positive responses in all animals. Irrigation of the eyes only slightly reduced the irritation potential.
Liggett and Parcell 1986b.

Source:
Reliability: (1) valid without restriction
21-FEB-2003 (42)

5.3 Sensitization

Type: other: sensitization
Species: guinea pig
Number of
Animals: 20
Vehicle: other: corn oil
Result: not sensitizing
Classification:
Method: other: Magnusson and Kligman
Year: 1969 **GLP:** yes
Test substance: other TS: Dobanic acid 103 (Benzenesulfonic acid, C10-13) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)

Remark: In a guinea-pig maximization test none of the test animals showed positive responses at 24 or 48 hours after removal of the challenge patches. The test material showed no sensitizing potential in guinea pigs.

Source: Rose 1983.
Reliability: (1) valid without restriction
21-JAN-2002 (44) (66)

Type: Guinea pig maximization test
Species: other: guinea pig, Hartley
Number of
Animals: 20
Vehicle: water
Result: not sensitizing
Classification: not sensitizing
Method: other: OECD Guideline 406; Directive 179/831 Annex, Part B.
Year: 1981 **GLP:** yes
Test substance: other TS: LAS, activity: 50%; average alkyl chain length = C11.6

Remark: Solutions of LAS were applied intracutaneously and epicutaneously to 10 male and 10 female animals. Induction concentration was 25% in water; the challenge concentration was 12.5%. No positive responses were observed.

Source: RBM 1985.
Reliability: (1) valid without restriction
21-FEB-2003 (64)

5.4 Repeated Dose Toxicity

Species: rat **Sex:** male/female
Strain: Wistar
Route of admin.: drinking water
Exposure period: 9 months
Frequency of treatment: Daily in drinking water
Post. obs. period:
Doses: 0.07, 0.2%, 0.6% (85, 145, 430 mg/kg bw d)
Control Group: yes
NOAEL: = 85 mg/kg bw
LOAEL: = 145
Method: other: Groups of 8-9 male and 8-9 female rats were given LAS for 9 months.
Year: **GLP:** no
Test substance: other TS: C10-14 LAS (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = C11.7
Remark: Information as cited in IPCS document. This study represents the most appropriate NOAEL value identified by the Industry Coalition for the SIDS Assessment of LAS (LAS Coalition). The LAS Coalition reviewed fifteen studies in which rodents (rats and mice) and non-rodents (monkeys) received repeated exposures to LAS via the oral or dermal routes. Test durations ranged from 15 days up to 9 months in those studies. LOAELs ranged from 115 to 750 mg/kg bwd and the highest NOAEL (below the lowest LOAEL) was found to be the 85 mg/kg bwd resulting from the study summarized here.
Result: Body weight gain was suppressed in the male 0.6% group. Haematological, serum-biochemical, and enzymatic parameters of the liver and kidney were also affected in the high dose groups. No organ weight changes were observed. The intake of LAS was 50 mg/kg bw d in the male 0.07% group. The values for the 0.2% group were 120 and 170 mg/kg bw d for males and females, respectively.
Source: European Commission 2000a; Yoneyama et al. 1976.
Reliability: (4) not assignable
21-MAR-2003 (12) (81)

5.5 Genetic Toxicity 'in Vitro'

Type: other: Bacterial reverse mutation assay (Ames test)
System of testing: Salmonella typhimurium TA 98 and TA 100
Concentration: 1.5 to 1500 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: Ames
Year: **GLP:** yes
Test substance: other TS: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: The test material was tested up to its toxic limit.
Result: No significant increases in the frequency of revertant colonies were recorded for either of the bacterial strains with any dose of the test substance, either with or without metabolic activation.
Source: Thompson 1998.
Reliability: (1) valid without restriction
05-NOV-2001 (72)

Type: Ames test
System of testing: Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, TA 100
Concentration: 8-5000 ug/plate
Metabolic activation: with and without
Result: negative
Method: Directive 84/449/EEC, B.14 "Other effects - Mutagenicity (Salmonella typhimurium - reverse mutation assay)"
Year: 1984 **GLP:** yes
Test substance: other TS: Marlon A 390 (CAS #68411-30-3) C10-13 LAS, average alkyl chain length = C11.6; activity 91.3%
Remark: Negative and positive controls used.
Result: Cytotoxicity concentration:
With metabolic activation: > 5000 ug/plate
Without metabolic activation: > 5000 ug/plate
Source: EEC Directive 1984; Schoeberl 1993a.
Reliability: (1) valid without restriction
21-FEB-2003 (8) (68)

Type: other: transformation test with SHE-cells
System of testing: Syrian hamster embryo (SHE) cells
Concentration: up to 50 ug/ml
Metabolic activation: without
Result: negative
Method:
Year: **GLP:** no
Test substance: other TS: C10-14 LAS, sodium salts (CAS #69669-44-9)
Method: Cell cultures were prepared and plated in 75 cm2 flasks containing 20 mL of culture medium. On day 5, target cells were trypsinized and a suspension of target cells was added to the solution plated on complete medium. Plates were dosed on day 6. Nine dishes were used for each dose level. On day 14, the cultures were fixed, stained, and examined to count normal and transformed colonies.
Remark: LAS did not produce transformation at any of the doses tested.
Source: Inoue et al. 1980.
Test substance: average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = C11.7; activity: 22.2%
Reliability: (2) valid with restrictions
21-FEB-2003 (26)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
Species: mouse **Sex:** male/female
Strain: NMRI
Route of admin.: other: oral intubation
Exposure period: 72 hours
Doses: 1122 mg/kg
Result: negative
Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year: 1983 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: No significant increases in the number of polychromatic erythrocytes with micronuclei were observed.
Source: Fedtke 1991; OECD 1983.
Reliability: (1) valid without restriction
11-OCT-2001 (13) (55)

Type: other: Mammalian bone marrow cytogenetic assay
Species: other: mouse: ICR: JCL **Sex:** male
Strain: ICR
Route of admin.: gavage
Exposure period: 5 days and 1 day
Doses: 200, 400, 800 mg/kg
Result: negative
Control Group: other: yes, concurrent no treatment, positive, and historical controls
Method: other: Chromosomal aberrations were examined 6, 24, 48 hours after administration. Mytomycin C was used as a positive control at a dose of 5 mg/kg and induced severe chromosomal aberrations.
Year: **GLP:** no
Test substance: other TS: C10-14 LAS, sodium salt (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = 11.7
Remark: Besides the pure LAS, commercial preparation containing 19% LAS and another containing 17.1% LAS were given to mice as single doses only by gavage at 800, 1600 or 3200 mg/kg bw d and 1000, 2000 or 4000 mg/kg bw d, respectively. The highest doses were 50% of the respective LD50 values. No significant differences in the incidence of chromosomal aberrations were observed in any LAS treatment relative to the controls. Information as cited in the IPCS document.
Result: There was no significant difference in the incidence of chromosomal aberrations between any of the groups given LAS and the negative control group.
Source: Inoue et al. 1977; European Commission 2000a.
Reliability: (4) not assignable
20-FEB-2003 (12) (25)

5.7 Carcinogenicity

Species: rat **Sex:** male/female
Strain: other: Charles River
Route of admin.: oral feed
Exposure period: 2 years
Frequency of treatment: continuous in feed
Post. obs. period:
Doses: 0.02, 0.1, 0.5% (10, 50, 250 mg/kg bw d)
Result:
Control Group: other: yes, concurrent no treatment and historical controls
Method:
Year: **GLP:** no
Test substance: other TS: C10-14 LAS, sodium salt (CAS# 69669-44-9); 98.1% activity on an anhydrous basis (41.9% active)
Method: Four groups of Charles River weanling rats, divided by sex, were given 0.5, 0.1, and 0.02% LAS in their food for 2 years. Following completion of those studies, five male and five female rats from each of the parental groups (F1b and F2b) and all survivors were selected for necropsy. Body weight and organ to body weight ratios were recorded, and routine hematology and histology were performed. Weanling animals for

Result: the F3a generation were similarly treated. Gross examination of all animals for pathology did not reveal any abnormalities. No consistent dietary induced changes that could be considered a toxic response were observed. Animals that showed significant loss of weight, development of tumors, or other evidence of abnormalities were sacrificed and tissues examined. The incidence of tumors and the common incidental diseases were similar in all dieting groups.

Source: Buehler et al. 1971.

Reliability: (2) valid with restrictions

27-MAR-2003 (2)

5.8 Toxicity to Reproduction

Type: other: 3-generation reproduction study

Species: rat **Sex:** male/female

Strain: other: Charles River

Route of admin.: oral feed

Exposure Period: 2 years

Frequency of treatment: continuous in feed

Premating Exposure Period

male: 84 days

female: 84 days

Duration of test: 3 generations

Doses: 0.02, 0.1, 0.5% (14, 70, 350 mg/kg bw d)

Control Group: yes

NOAEL Parental: = 350 mg/kg bw

NOAEL F1 Offspr.: = 350 mg/kg bw

NOAEL F2 Offspr.: = 350 mg/kg bw

Method:

Year: 1971 **GLP:** no

Test substance: other TS: Sodium salt LAS (C10-14), activity: 98.1% on an anhydrous basis (41.9% active)

Method: Na-LAS (chain length distribution C10-14) was fed for 84 days to 4 groups of weanling rats (3 dose levels, plus control), each dose consisting of 50 animals each of both sexes (P0-generation). When the P0 generation was 107-112 days old, 20 females from each dose group were mated with 20 males from the same group and maintained together for 17 days. The first litters of each generation (Fla- and F2a-generation) were sacrificed at 21 days of age. Ten days after the final litter was sacrificed, all females were remated with different males from the same group to obtain the Flb generation. From the Flb-generation, 20 males and females of each group were selected at weaning to continue their respective diets and to be used for further reproduction studies. Reproduction studies on the Flb and F2b generations were started when the rats were 80 to 85 days old, and were continued until the F3b generation was weaned.

Result: Results were reported as no effects at the highest

concentration tested (0.5% in the diet). General reproduction including fertility gestation, parturition, neonatal viability, lactation, and post-weaning growth was normal for all test groups and did not deviate from the controls in each generation. No gross abnormalities were noted. No definitive adverse effects due to the test material were noted in the haematology and pathology.

Source: Buehler et al. 1971.
Reliability: (2) valid with restrictions
20-FEB-2003

(2)

5.9 Developmental Toxicity/Teratogenicity

Species: rat **Sex:** female
Strain: other: SD-JCL
Route of admin.: oral feed
Exposure period: from day 0 to 20 of gestation
Frequency of treatment: daily
Duration of test:
Doses: 0.1%, 1.0% (80, 780 mg/kg bw d)
Control Group: yes
NOAEL Maternalt.: = 780 mg/kg bw
NOAEL Teratogen.: = 780 mg/kg bw
Method: other: LAS was fed in the diet to 16 pregnant female rats/dose from day 0 to 20 of gestation.
Year: **GLP:** no
Test substance: other TS: Japan LAS; average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = C11.7-12.3.
Remark: Information as cited in IUCLID Data Sheet and IPCS document. This study represents the most appropriate NOAEL value identified by the Industry Coalition for the SIDS Assessment of LAS. The LAS Coalition reviewed ten developmental toxicity studies conducted on rats, mice and rabbits in which the test animals received LAS via the oral route (feed, gavage, or drinking water). While effects were observed at maternally toxic doses, no decreases in litter size, no changes in litter parameters, and no malformations or significant differences in skeletal defects were observed in these studies at oral doses up to 780 mg/kg bwd. Note also that the NOAEL used in the risk assessment is derived from the repeated dose studies.
Result: The LAS intake was about 780 mg/kg with the 1% diet, but there were no abnormalities in the body weight gains of the dams, or in the occurrence and maintenance of pregnancy. The values of the litter parameters did not differ from those of the controls and there was no evidence of teratogenicity. The numbers of offspring were rather low in the 1% group, and the weaning rate of 78.3% was lower than the 100% rate observed in the controls. However, there were no abnormalities in body weight gain, organ weights or functions in the offspring.
Source: European Commission 2000a; Tiba et al. 1976.
Reliability: (4) not assignable
21-MAR-2003

(12) (73)

Species: mouse **Sex:** female
Strain: ICR
Route of admin.: dermal
Exposure period: from day 6 through day 15 of pregnancy
Frequency of treatment: daily
Duration of test:
Doses: 0.03, 0.3, 3% (15, 150, and 1500 mg/kg bw d)
Control Group: yes
NOAEL Maternalt.: = 150 mg/kg bw
NOAEL Teratogen.: = 1500 mg/kg bw
Method: other: Areas of 4 x 4 cm on the backs of the mice were depilated and aqueous solutions of LAS were applied.
Year: **GLP:** no
Test substance: other TS: C10-14 LAS (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = C11.7; activity: 46.6%
Remark: Information as cited in the IUCLID Data Sheet and the IPCS document. This study represents the most appropriate NOAEL value identified by the Industry Coalition for the SIDS Assessment of LAS. The LAS Coalition reviewed seven developmental toxicity studies conducted on rats, mice and rabbits in which the test animals received LAS via the dermal route. While effects were observed at maternally toxic doses, no decreases in litter size, no changes in litter parameters, and no malformations or significant differences in skeletal defects were observed in these studies at dermal doses up to 1,500 mg/kg bwd. Note also that the NOAEL used in the risk assessment is derived from the repeated dose studies.
Result: The 3% group showed a clear decrease in the pregnancy rate (67.9%) when compared with a rate of 96.3% in the controls. However, there were no decreases in the litter size, and no changes in the litter parameters with the exception of a slight decrease in fetal body weight. There were no significant increases in the incidence of malformations in the fetuses.
Source: European Commission 2000a; Imahori et al. 1976.
Reliability: (4) not assignable
21-MAR-2003 (12) (24)

5.10 Other Relevant Information

Type:
Remark: None
11-OCT-2001

5.11 Experience with Human Exposure

Memo: LAS has been extensively studied and used for many years without significant incidents.
11-OCT-2001

-
- (1) 49 CFR 173.1200 Appendix A. Method of testing corrosion to the skin.
 - (2) Buehler, E.V., Newmann, E.A., and King, W.R. 1971. Two year feeding and reproduction study in rats with linear alkylbenzene sulfonate (LAS). Toxicol. Appl. Pharmacol. 18:83-91.
 - (3) Cohen, L., Vergara, R., Moreno, A. and Berna, J.L. 1995. Influence of 2-phenyl alkane and telralin content on solubility and viscosity of linear alkylbenzene sulfonate. JAOCS 72:115-122.
 - (4) CONDEA Vista. 1995. Material Safety Data Sheet for VISTA SA-597L Sulfonic Acid, Revision No. 02/95, last revised 4/24/95.
 - (5) Cross, J. and Dekker, M. (ed.). 1977. Anionic surfactants: Chemical analysis, v. 8, p. 111-115.
 - (6) Deutsche Einheitsverfahren zur Wasser-, Abwasser- und Schlamm-untersuchung. L 11: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Kleinkrebse (Daphnien-Kurzzeittest). DIN 38412 Teil 11.
 - (7) Deutsche Einheitsverfahren zur Wasser-, Abwasser-, und Schlammuntersuchung. L 15: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Fische - Fischtest DIN 38412 Teil 15.
 - (8) Directive 84/449/EEC, B.14 mutagenicity. 1984. Salmonella typhimurium-reverse mutation assay.
 - (9) Directive 84/449/EEC, C.2. 1984. Acute toxicity for Daphnia.
 - (10) Douglas, M.T., Chanter, D.O., Pell, I.B., and Burney, G.M. 1986. A proposal for the reduction of animal numbers required for the acute toxicity to fish test (LC50 determination). Aquat. Toxicol. 8:243-249.
 - (11) Draize, J.H. 1965. Appraisal of the safety of chemicals in foods, drugs, and cosmetics-dermal toxicity. Association of Food and Drug Officials of the U.S., Topeka, Kansas Pp. 46-59.
 - (12) European Commission. 2000a. Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.

-
- (13) Fedtke, N. 1991. Mutagenitätsprüfung von Marlon AS 3 im in vivo mikrokerntest an der maus. Report No. MK-91/0026.
- (14) Freitag, D., Ballhorn, L., Geyer, H., and Korte, F. 1985. An experimental method for the assessment of the behaviour of organic chemicals in the ecosphere by means of simple laboratory tests with C14 labelled chemicals. Chemosphere 14:1589-1616.
- (15) Galassi et al. 1992. Water Res. 26:19-27 as cited in IUCLID. 1995. IUCLID data sheet: dodecylbenzenesulfonic acid.
- (16) Hand, V.C. and Williams, G.K. 1987. Structure-activity relationships for sorption of linear alkylbenzenesulfonates. Environ. Sci. Technol. 21:370-373.
- (17) Hempstock, C. 1998. NEOPELEX FS: Acute oral toxicity study in the rat - Acute toxic class method. SPL Project No. 140/854.
- (18) HERA. 2002. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. 68411-30-3, Draft #6, May 2002.
- (19) Hoechst AG. 1988. Unveröffentlichte unters. ber. 88.0913. as cited in IUCLID. 1995. IUCLID data sheet: dodecylbenzenesulfonic acid.
- (20) Hoechst AG. 1988. Unveröffentlichte unters. ber. 88.0925. as cited in IUCLID. 1995. IUCLID data sheet: dodecylbenzenesulfonic acid.
- (21) Huels. 1993. Huels report No. DDA-21.
- (22) Huntsman 2002. Report on the melting point analysis for NANSA HS 85/S. Attached technical bulletin dated 04-01-1994. Cover memo from A. Ashworth to K.B. Sellstrom dated April 12, 2002.
- (23) Huntsman. 2002. Report of melting point analysis for NANSA HS 85/5. Cover memo from A. Ashworth to K.B. Sellstrom dated April 12, 2002.
- (24) Imahori, A., Kinagawa, T. and Shiobara, S. 1976. Effects of linear alkyl benzene sulfonate (LAS) applied dermally to pregnant mice and their fetuses. Jpn. J. Public Health. 23:68-72 (in Japanese); cited in IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

-
- (25) Inoue, K., Shibata, T., Hamano, Y., Oda, Y., Kuwano, A., Yamamoto, H., Mitsuda, B. and Kunita, N. 1977. In vivo cytogenetic tests of some synthetic detergents in mice. Ann Res. Osaka Prefect Inst. Public Health. 8:17-24 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
- (26) Inoue, K., Sunakawa, T., and Takayama. 1980. Studies of in vitro cell transformation and mutagenicity by surfactants and other compounds. Fd. Cosmet. Toxicol. 18:289-296.
- (27) IUCLID. 1995. IUCLID data sheet: Benzenesulfonic acid, C10-16-alkyl derivatives.
- (28) IUCLID. 1995. IUCLID data sheet: Dodecylbenzenesulphonic acid.
- (29) Kinney, L.A. 1985. Approximate lethal concentrations (ALCs) by inhalation of sodium lauryl sulfate & sodium dodecylbenzene sulfonate. Dupont Haskell Laboratory Report No. 474-84.
- (30) Knie, V.J., Halke, A., Juhnke, I., and Schiller, W. 1983. Ergebnisse der untersuchungen von chemischen stoffen mit vier biotests (Results of studies on chemical substances with four biotests). Deutsch Gewasserkundliche Mitteilungen 77-79.
- (31) Kretchmar. 1972. Acute toxicity studies with XTW-1226. Report to Procter & Gamble Company, IBT No. A1717.
- (32) Kurtin. 1994. Bestimmung der Auswirkungen von Marlon AS 3 auf das wachstum von Scenedesmus subscipicatus 86.81.SAG. Report No. AW-371.
- (33) Kurtin. 1994. Bestimmung der biologischen Abbaubarkeit von Marlon AS 3 im DOC-Die-Away test. Report No. DDA-79.
- (34) Kurtin. 1994. Bestimmung der biologischen Abbaubarkeit von Marlon AS 3 im modifizierten coupled units-test. Report No. MCU-21.
- (35) Kurtin. 1995. Bestimmung der auswirkungen von MARLON AS 3 auf das schwimmverhalten von Daphnia magna. Report No. DK-620.
- (36) Kurtin. 1997. Bestimmung der akuten wirkungen von MARLON AS 3 gegenuber fischen. Report No. FK-1375.

-
- (37) Kynoch, S.R. 1986a. Acute oral toxicity to rats: P-500 N-Na. Huntingdon Research Center Report. No. 86546D/PEQ 7/AC.
- (38) Kynoch, S.R. 1986b. Acute dermal toxicity to rats of P-500 N-Na. Huntingdon Research Center. Report No. 86718D/PEQ 8/AC.
- (39) Leo, A.J. and Hansch, C. 1979. Substituent Constants for Correlation Analysis in Chemistry and Biology. J. Wiley & Sons, N.Y.
- (40) Lide, D.R. 1990. Handbook of Chemistry and Physics. 71st Edition. CRC Press: Ann Arbor.
- (41) Liggett, M.P. and Parcell, B.I. 1986a. Irritant effects on rabbit skin of P-500 N-Na. Huntingdon Research Center. Report No. 86400D/PEQ 9/SE.
- (42) Liggett, M.P. and Parcell, B.I. 1986b. Irritant effects on the rabbit eye of P-500 N-Na. Huntingdon Research Center Report No. 86570D/PEQ 10/SE.
- (43) Lyman, W.J. 1985. Environmental exposure from chemicals, V.I, p.31, Neely, W.B., and Blau, G.E., editors. CRC Press. Boca Raton.
- (44) Magnusson, B. and Kligman, A.M. 1969. The identification of contact allergens by animal assay: The guinea pig maximization test. J. Invest. Dermatol. 52:268-276.
- (45) Matsuura, T. and Smith, J.M. 1970. Kinetics of photodecomposition of dodecyl benzene sulfonate. Ing. Eng. Chem. Fund. 9:252-260.
- (46) Murmann, P. 1984. Acute orale Toxizität von Marlon AS 3-Saure für Ratten. Report No. 0303.
- (47) Murmann, P. 1984. Prüfung der akuten augen- und schleimhautreizwirkung von Marlon AS 3-saure. Report No. 0305.
- (48) Murmann, P. 1984. Prüfung der akuten hautreizwirkung von Marlon AS 3-Saure. Report No. 0304.
- (49) Murmann, P. 1984a. Akute orale Toxizität von Marlon A 386 für Ratten. Huels Report No. 0191.
- (50) Noeller, C.R. 1966. Textbook of Organic Chemistry. 3rd Edition. W.B. Saunders Company: Philadelphia.

-
- (51) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals 305E.
 - (52) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals No. 401.
 - (53) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals No. 404.
 - (54) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals No. 405.
 - (55) Organisation for Economic Co-operation and Development (OECD). 1983. OECD guidelines for the testing of chemicals No. 474.
 - (56) Organisation for Economic Co-operation and Development (OECD). 1984. OECD guidelines for the testing of chemicals No. 201.
 - (57) Organisation for Economic Co-operation and Development (OECD). 1984. OECD guidelines for the testing of chemicals No. 202.
 - (58) Organisation for Economic Co-operation and Development (OECD). 1984. OECD guidelines for the testing of chemicals, No. 203.
 - (59) Organisation for Economic Co-operation and Development (OECD). 1987. OECD guidelines for the testing of chemicals, No. 401.
 - (60) Organisation for Economic Co-operation and Development (OECD). 1992. OECD guidelines for the testing of chemicals, No. 203.
 - (61) Organisation for Economic Co-operation and Development (OECD). 1992. OECD guidelines for the testing of chemicals, No. 301B.
 - (62) Organisation for Economic Co-operation and Development (OECD). 1995. OECD guidelines for the testing of chemicals, No. 202.
 - (63) Procter & Gamble. 1991. AT/17.

-
- (64) RBM. 1985. Test di sensibilizzazione cutanea nella cavia. RBM Exp. No. 2076.
- (65) Roberts, D.W. 1991. QSAR issues in aquatic toxicity of surfactants. Sci. Total Environ. 109/110:557-568.
- (66) Rose, G.P. 1983. Toxicology of detergents: The skin sensitizing potential of Dobanic acid 103. Group research report SBGR.83.383.
- (67) Schoeberl, P. 1991. Coupling the OECD confirmatory-test with continuous ecotoxicity tests. Communication 1: Modification of the OECD confirmatory test (sewage treatment plant simulation model). Tenside Surfactants Detergents 6.
- (68) Schoeberl, P. 1993a. Bestimmung der Mutagenitat von Marlon A 390 im Salmonella/Sauger-Mikrosomen-Mutagenitatstest nach Ames. Huels Final Report No. AM-93/12.
- (69) Stepan Company. Biotic degradation (modified Sturm test) evaluation, in an aqueous medium, of the "ultimate" biodegradability of substances: 1736-1A, 1736-1B, 1736-1C, 1736-1D, 1736-1E. Ineris-Study 16 BF 53.
- (70) Stephenson, R.R. 1981. Dobanic acid 102: Acute toxicity to Salmo gairdneri, Daphnia magna, and Selenstrum capricornutum. Group research preport SBGR.81.083.
- (71) Thompson, G.W. 1980. D.O.T. skin corrosivity-method, summary for Bio-Soft S-100. Raltech Scientific Services. Lab Study No. 793159.
- (72) Thompson, P.W. 1998. NEOPELEX FS: Reverse mutation assay "Ames test" using Salmonella typhimurium strains TA 98 and TA 100 - single experiment. SLP Project No. 140/855.
- (73) Tiba, S., Shiobara, S., Imahori, A. and Kitagawa, T. 1976. Effects of linear alkylbenzene sulfonate on dam, fetus and newborn rat. J. Food Hyg. Soc. Jpn. 17:66-71. (In Japanese); cited in IPCS. 1996. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates and Related Compounds. World Health Organization, Geneva, Switzerland. Original article in Japanese.
- (74) Tolls, J., Haller, M., DeGraaf, I., Thijssen, M.A.T.C., and Sijm, D.T.H.M. 1997. Bioconcentration of LAS: Experimental determination and extrapolation to environmental mixtures. Environ. Sci. Technol. 31:3426-3431.

-
- (75) USEPA 1985.
- (76) USEPA. 2000. EpiSuite Estimation Software V.3.10. US Environmental Protection Agency.
- (77) van de Plassche, E.J., DeBruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J., and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: Linear alkyl benzene sulfonate, alcohol ethoxylates, alcohol ethoxylated sulfates, and soap. Environ. Toxicol. Chem. 18: 2653-2663.
- (78) Verge, C. and Moreno, A. 1996. Toxicity of anionic surfactants to green microalgae "Scenedesmus subspicatus" and "Selenastrum capricornutum". Tenside Surf. Det. 33:166-168.
- (79) Verge, C. and Moreno, A. 2000. Effects of anionic surfactant on Daphnia magna. Tenside Surf. Det. 37:172-175.
- (80) Verschueren, K. 1996. Handbook of Environmental Data on Organic Chemicals, Third Edition. New York: John Wiley & Sons, Inc.
- (81) Yoneyama, M., Mabuchi, Y., Ikawa, M., Kobayashi, H. and Ichikawa, H. 1976. Subacute toxicity of linear alkylbenzene sulfonate. Ann. Rep. Tokyo Metr. Res. Lab. Public Health 27:105-112 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO Geneva, Switzerland.

7.1 Risk Assessment

Memo: See LAB sulfonic acids assessment plan.
21-MAR-2003